Jan Delaval.

Access DB# 120099

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Sabiha Qazi Examiner #: 74141 Date: 4/21/04
Art Unit: 1616 Phone Number 30 20622 Serial Number: 09/619,584
Mail Box and Bldg Room Location: 4-C70 Rem 4A45 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need. MEJ

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc. if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Bicyclic Arom. Compds

Inventors (please provide full names): Bernardon, Jean-Michel

Earliest Priority Filing Date: 1/26/1998 (See US 6,147,255)

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please search for the compds. of Clm 33

Please see attached sheet

Thank you

****

STAFF USE ONLY		Type of Search		Vendors and cost where applicable	
Searcher	Jan	NA Sequence (#)		STN	✓
Searcher Phone #	22504	AA Sequence (#)		Dialog	
Searcher Location:		Structure (#)	✓	Questel/Orbit	
Date Searcher Picked Up	4/22	Bibliographic		Dr.Link	
Date Completed:	4/22	Litigation		Lexis/Nexis	
Searcher Prep & Review Time:		Fulltext		Sequence Systems	
Clerical Prep Time	20	Patent Family		WWW/Internet	
Online Time	175	Other		Other (specify)	

PTO-1590 (8-01)

Access DB # 120099


```
=> fil reg
FILE 'REGISTRY' ENTERED AT 13:58:43 ON 22 APR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   21 APR 2004  HIGHEST RN 676437-01-7
DICTIONARY FILE UPDATES:  21 APR 2004  HIGHEST RN 676437-01-7

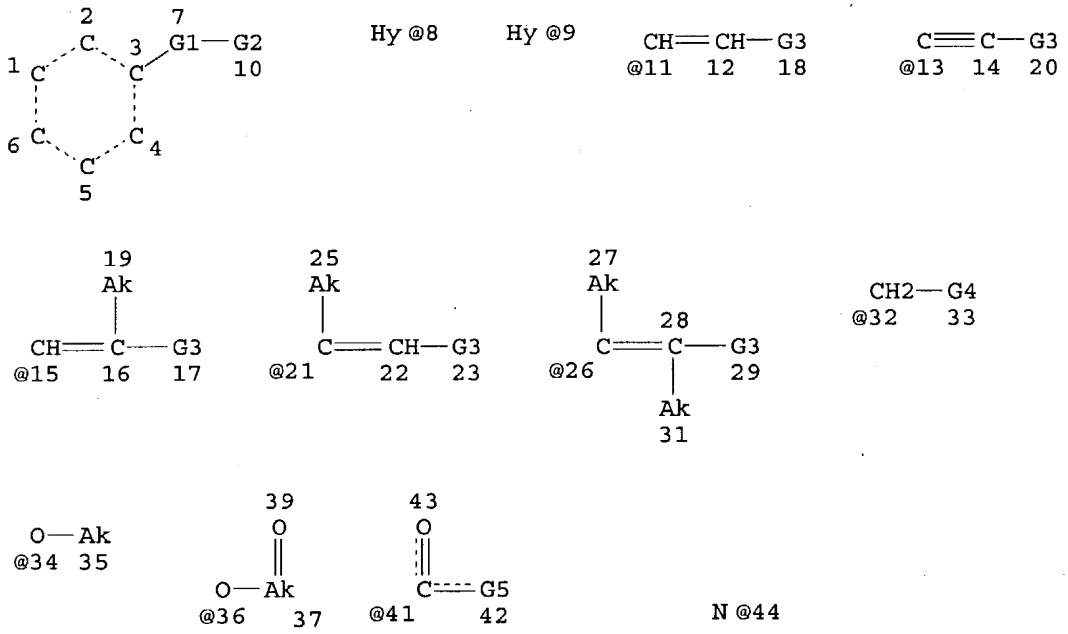
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d sta que l44
L1                STR
```

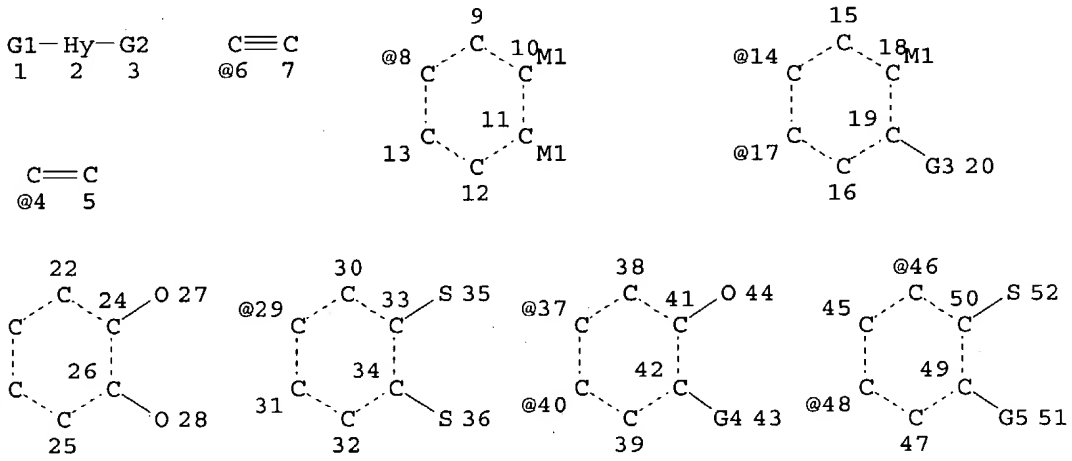



```
VAR G1=8/9
VAR G2=11/13/15/21/26
VAR G3=ME/32/41
VAR G4=OH/34/36
VAR G5=H/AK/44
NODE ATTRIBUTES:
CONNECT IS M1  RC AT   1
CONNECT IS M1  RC AT   2
CONNECT IS M1  RC AT   4
CONNECT IS M1  RC AT   5
CONNECT IS M1  RC AT   6
CONNECT IS M1  RC AT  44
```

```
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  AT   8
GGCAT   IS MCY  AT   9
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 O  AT   8
ECOUNT  IS E4 C  E1 S  AT   9

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  40

STEREO ATTRIBUTES: NONE
L3      1038332 SEA FILE=REGISTRY ABB=ON  PLU=ON  (SC4 OR OC4)/ES AND NR>=2
L6         4782 SEA FILE=REGISTRY SUB=L3 SSS FUL L1
L7          818 SEA FILE=REGISTRY SUB=L6 CSS FUL L1
L9              STR
```




```
VAR G1=4/6
VAR G2=8/14/21/29/37/40/46/48/17
VAR G3=O/S
VAR G4=S/H
VAR G5=O/H
NODE ATTRIBUTES:
HCOUNT  IS M1     AT  10
HCOUNT  IS M1     AT  11
HCOUNT  IS M1     AT  18
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  AT   2
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   8  14  21  29  37  45
NUMBER OF NODES IS  52

STEREO ATTRIBUTES: NONE
L11         413 SEA FILE=REGISTRY SUB=L7 SSS FUL L9
L12         405 SEA FILE=REGISTRY ABB=ON  PLU=ON  L7 NOT L11
L13             STR
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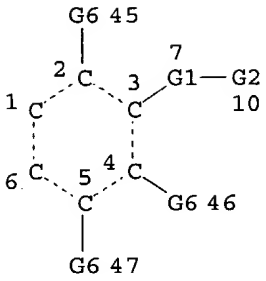
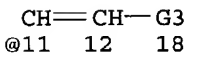
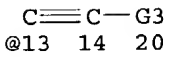
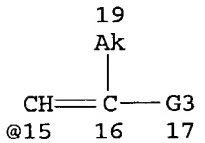


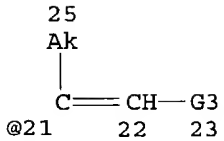
Hy @8

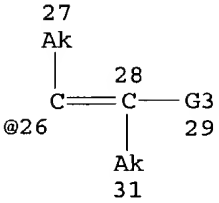
Hy @9

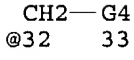


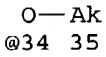


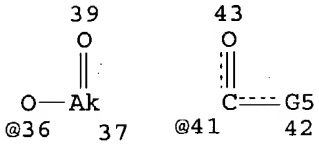










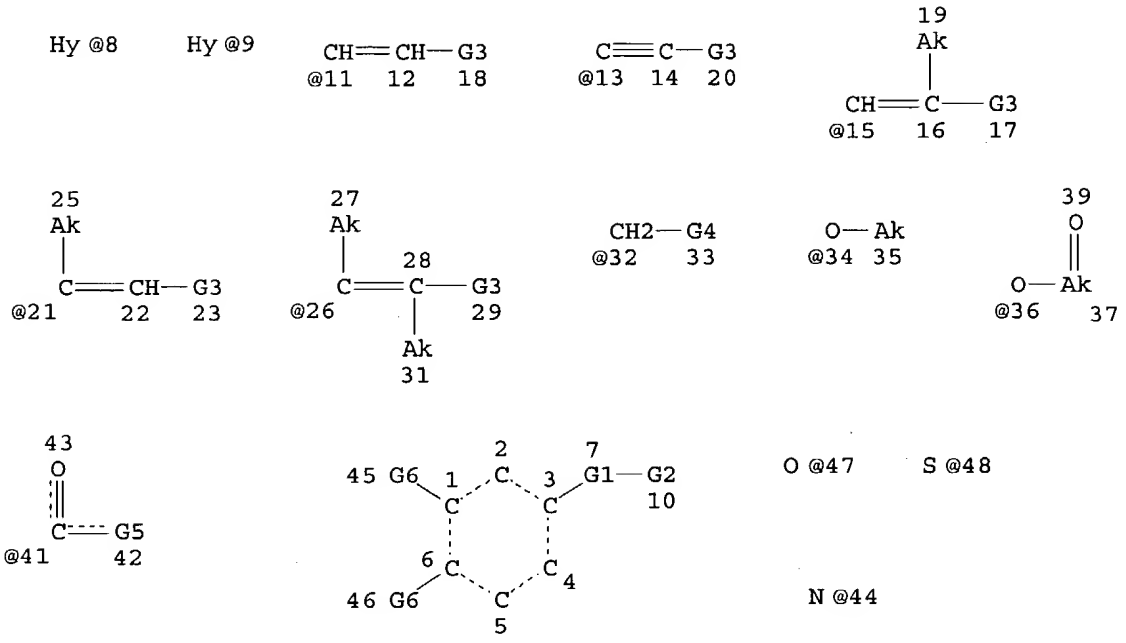


N @44

VAR G1=8/9
VAR G2=11/13/15/21/26
VAR G3=ME/32/41
VAR G4=OH/34/36
VAR G5=H/AK/44
VAR G6=H/X/AK/OH/34/36
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 1
CONNECT IS M1 RC AT 6
CONNECT IS M1 RC AT 44
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY AT 8
GGCAT IS MCY AT 9
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E1 O AT 8
ECOUNT IS E4 C E1 S AT 9

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 43

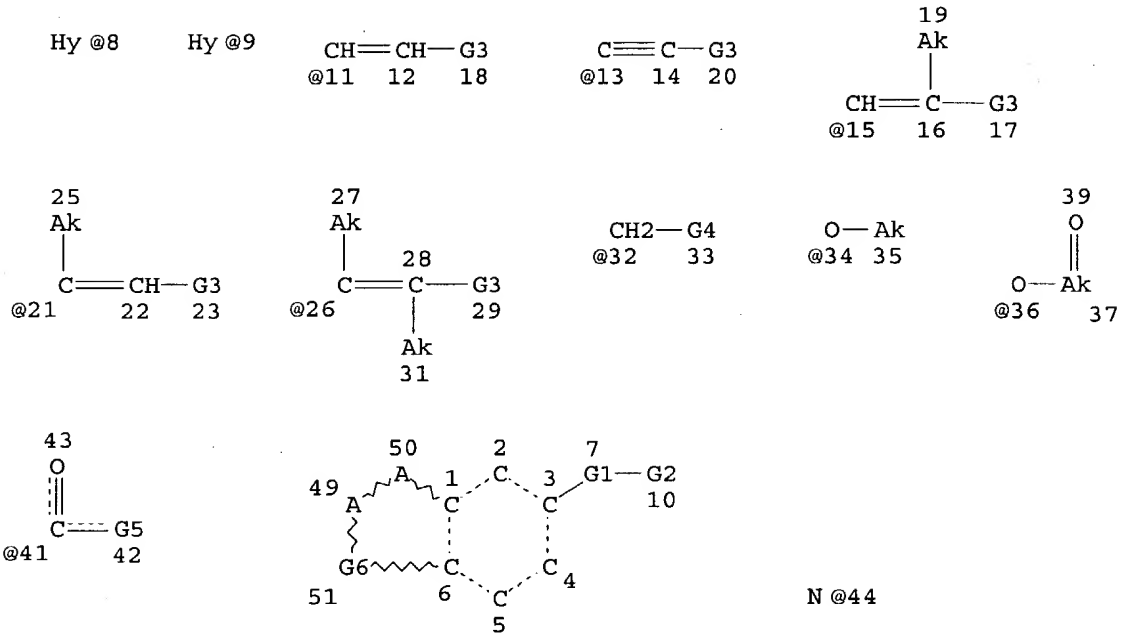
STEREO ATTRIBUTES: NONE
L15 397 SEA FILE=REGISTRY SUB=L12 CSS FUL L13
L17 STR



VAR G1=8/9
VAR G2=11/13/15/21/26
VAR G3=ME/32/41
VAR G4=OH/34/36
VAR G5=H/AK/44
VAR G6=H/AK/47/48
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 2
CONNECT IS M1 RC AT 4
CONNECT IS M1 RC AT 5
CONNECT IS M1 RC AT 44
CONNECT IS M1 RC AT 47
CONNECT IS M1 RC AT 48
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY AT 8
GGCAT IS MCY AT 9
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E1 O AT 8
ECOUNT IS E4 C E1 S AT 9

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 44

STEREO ATTRIBUTES: NONE
L18 26 SEA FILE=REGISTRY SUB=L15 CSS FUL L17
L19 6 SEA FILE=REGISTRY ABB=ON PLU=ON L18 AND (C39H36N2O4 OR C30H37N2O2S OR C28H32NO2PS OR C29H34NO2PS OR C29H34N2O2S OR C30H36N2O2S)
L20 STR



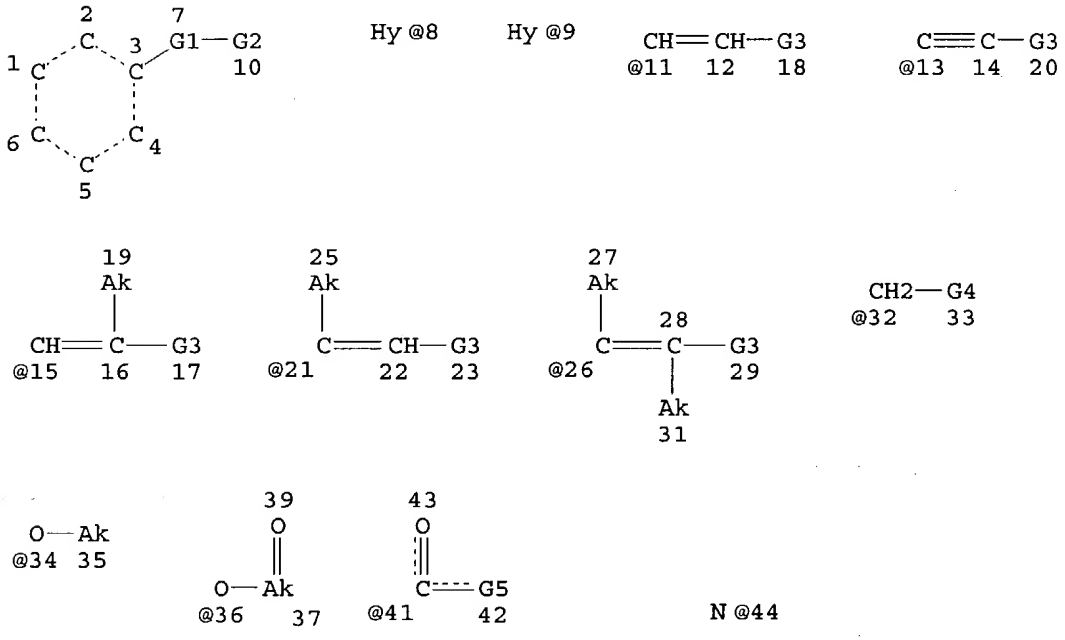

```
VAR G1=8/9
VAR G2=11/13/15/21/26
VAR G3=ME/32/41
VAR G4=OH/34/36
VAR G5=H/AK/44
REP G6=(1-2) A
NODE ATTRIBUTES:
CONNECT IS M1  RC AT   2
CONNECT IS M1  RC AT   4
CONNECT IS M1  RC AT   5
CONNECT IS M1  RC AT  44
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  AT   8
GGCAT   IS MCY  AT   9
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 O  AT   8
ECOUNT  IS E4 C  E1 S  AT   9

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  43

STEREO ATTRIBUTES: NONE
L22           6 SEA FILE=REGISTRY SUB=L15 SSS FUL L20
L28         124 SEA FILE=REGISTRY ABB=ON  PLU=ON  (108-40-7/BI OR 110-91-8/BI
                OR 1122-91-4/BI OR 119999-22-3/BI OR 1200-07-3/BI OR 123-30-8/B
                I OR 135631-86-6/BI OR 14804-34-3/BI OR 158115-92-5/BI OR
                168082-41-5/BI OR 168082-64-2/BI OR 169126-63-0/BI OR 169126-64
                -1/BI OR 170100-73-9/BI OR 170355-38-1/BI OR 1761-61-1/BI OR
                18791-75-8/BI OR 189698-90-6/BI OR 189698-91-7/BI OR 189699-37-
                4/BI OR 191469-48-4/BI OR 196960-59-5/BI OR 196960-60-8/BI OR
                196960-61-9/BI OR 196960-62-0/BI OR 196960-63-1/BI OR 196960-64
                -2/BI OR 196960-65-3/BI OR 196960-66-4/BI OR 196960-67-5/BI OR
                196960-68-6/BI OR 196960-69-7/BI OR 196960-70-0/BI OR 196960-71
                -1/BI OR 196960-72-2/BI OR 196960-73-3/BI OR 196960-74-4/BI OR
                196960-75-5/BI OR 196960-76-6/BI OR 196960-77-7/BI OR 196960-78
                -8/BI OR 196960-79-9/BI OR 196960-80-2/BI OR 196960-81-3/BI OR
```

196960-82-4/BI OR 196960-83-5/BI OR 196960-84-6/BI OR 196960-85
-7/BI OR 196960-86-8/BI OR 196960-87-9/BI OR 196960-88-0/BI OR
196960-89-1/BI OR 196960-90-4/BI OR 196960-91-5/BI OR 196960-92
-6/BI OR 196960-93-7/BI OR 196960-94-8/BI OR 196960-95-9/BI OR
196960-96-0/BI OR 196960-97-1/BI OR 196960-98-2/BI OR 196960-99
-3/BI OR 196961-00-9/BI OR 196961-01-0/BI OR 196961-02-1/BI OR
196961-03-2/BI OR 196961-04-3/BI OR 196961-05-4/BI OR 196961-06
-5/BI OR 196961-07-6/BI OR 196961-08-7/BI OR 196961-09-8/BI OR
196961-10-1/BI OR 196961-11-2/BI OR 196961-12-3/BI OR 196961-13
-4/BI OR 196961-14-5/BI OR 196961-15-6/BI OR 196961-16-7/BI OR
196961-17-8/BI OR 196961-18-9/BI OR 196961-19-0/BI OR 196961-20
-3/BI OR 196961-21-4/BI OR 196961-22-5/BI OR 196961-23-6/BI OR
196961-24-7/BI OR 196961-25-8/BI OR 196961-26-9/BI OR 196961-27
-0/BI OR 196961-28-1/BI OR 196961-29-2/BI OR 196961-30-5/BI OR
196961-31-6/BI OR 196961-32-7/BI OR 196961-33-8/BI OR 196961-34
-9/BI OR 196961-35-0/BI OR 196961-36-1/BI OR 196961-37-2/BI OR
19

L29 32 SEA FILE=REGISTRY ABB=ON PLU=ON L28 AND (OC4 OR SC4)/ES
L30 28 SEA FILE=REGISTRY ABB=ON PLU=ON L29 AND NR>=2
L31 11 SEA FILE=REGISTRY ABB=ON PLU=ON L30 AND (C22H26O2S OR
C20H24O3S OR C18H20O3S OR C22H26O2S OR C18H20O3S OR C20H26O3S
OR C24H30O2S OR C24H30O2S OR C21H24O2S OR C20H24O3S OR
C23H28O2S)
L32 STR



VAR G1=8/9
VAR G2=11/13/15/21/26
VAR G3=ME/32/41
VAR G4=OH/34/36
VAR G5=H/AK/44/OH/34
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 1
CONNECT IS M1 RC AT 2
CONNECT IS M1 RC AT 4
CONNECT IS M1 RC AT 5
CONNECT IS M1 RC AT 6
CONNECT IS M1 RC AT 44
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY AT 8

```
GGCAT   IS MCY  AT   9
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 O  AT   8
ECOUNT  IS E4 C  E1 S  AT   9

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  40

STEREO ATTRIBUTES: NONE
L34          946 SEA FILE=REGISTRY SUB=L3 CSS FUL L32
L35          128 SEA FILE=REGISTRY ABB=ON  PLU=ON  L34 NOT L7
L36           62 SEA FILE=REGISTRY SUB=L35 SSS FUL L9
L37           11 SEA FILE=REGISTRY ABB=ON  PLU=ON  L30 AND L35
L38           11 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L31 OR L37)
L39           57 SEA FILE=REGISTRY ABB=ON  PLU=ON  L36 NOT L38
L40           12 SEA FILE=REGISTRY ABB=ON  PLU=ON  L39 AND (C13H9CLO3 OR
                 C13H8CL2O3 OR C13H9BRO3 OR C18H20O3S OR C14H11CLO3 OR C13H8CL2O
                 3 OR C16H13CLO3 OR C18H20O3S)
L41           60 SEA FILE=REGISTRY ABB=ON  PLU=ON  L35 NOT (L38 OR L39 OR L40)
L42            5 SEA FILE=REGISTRY ABB=ON  PLU=ON  L41 AND (C18H16O2S OR
                 C17H18O2S OR C21H24O3 OR C23H28O3 OR C18H20O2S)
L43           40 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L19 OR L22 OR L38 OR L40 OR
                 L42)
L44           36 SEA FILE=REGISTRY ABB=ON  PLU=ON  L43 NOT QUINAZOL?


=> d his

     (FILE 'HOME' ENTERED AT 12:50:26 ON 22 APR 2004)
                SET COST OFF

     FILE 'REGISTRY' ENTERED AT 12:50:36 ON 22 APR 2004
L1                STR
L2              0 S L1 CSS
L3        1038332 S (SC4 OR OC4)/ES AND NR>=2
L4              5 S L1 CSS SAM SUB=L3
L5             21 S L1 SAM SUB=L3
L6           4782 S L1 FUL SUB=L3
                  SAV L6 QAZI619/A TEMP
L7            818 S L1 CSS FUL SUB=L6
                  SAV TEMP L7 QAZI619A/A

     FILE 'HCAOLD' ENTERED AT 13:00:22 ON 22 APR 2004
L8              5 S L7

     FILE 'REGISTRY' ENTERED AT 13:07:05 ON 22 APR 2004
L9                STR
L10            16 S L9 SAM SUB=L7
L11           413 S L9 FUL SUB=L7
                  SAV L11 QAZI619B/A
L12           405 S L7 NOT L11
L13               STR L1
L14            18 S L13 CSS SAM SUB=L12
L15           397 S L13 CSS FUL SUB=L12
                  SAV L15 QAZI619C/A
L16               STR L13
L17               STR L16
L18            26 S L17 CSS FUL SUB=L15
                  SAV L18 QAZI619D/A
L19             6 S L18 AND (C39H36N2O4 OR C30H37N2O2S OR C28H32NO2PS OR C29H34NO
L20               STR L17
L21             0 S L20 SAM SUB=L15
```

```
L22           6 S L20 FUL SUB=L15
                SAV L22 QAZI619E/A

     FILE 'HCAOLD' ENTERED AT 13:25:53 ON 22 APR 2004
L23           0 S L19 OR L22

     FILE 'HCAPLUS' ENTERED AT 13:25:56 ON 22 APR 2004
L24           5 S L19 OR L22
                E BERNARDON J/AU
L25          68 S E4-E7
                E GALDERM/PA,CS
L26         169 S E3-E38
L27           1 S (FR96-3235 OR WO97-FR391)/AP,PRN OR (US6147255 OR US6515021 O
                SEL RN

     FILE 'REGISTRY' ENTERED AT 13:28:27 ON 22 APR 2004
L28         124 S E1-E124
L29          32 S L28 AND (OC4 OR SC4)/ES
L30          28 S L29 AND NR>=2
L31          11 S L30 AND (C22H26O2S OR C20H24O3S OR C18H20O3S OR C22H26O2S OR
L32             STR L1
L33           6 S L32 CSS SAM SUB=L3
L34         946 S L32 CSS FUL SUB=L3
                DEL QAZI619?/A
                SAV L34 QAZI619A/A
L35         128 S L34 NOT L7
L36          62 S L9 FUL SUB=L35
                SAV L36 QAZI619B/A
L37          11 S L30 AND L35
L38          11 S L31,L37
L39          57 S L36 NOT L38
L40          12 S L39 AND (C13H9CLO3 OR C13H8CL2O3 OR C13H9BRO3 OR C18H20O3S OR
L41          60 S L35 NOT L38-L40
L42           5 S L41 AND (C18H16O2S OR C17H18O2S OR C21H24O3 OR C23H28O3 OR C1
L43          40 S L19,L22,L38,L40,L42
L44          36 S L43 NOT QUINAZOL?
                SAV QAZI619C/A L44

     FILE 'HCAOLD' ENTERED AT 13:57:48 ON 22 APR 2004
L45           0 S L44

     FILE 'HCAPLUS' ENTERED AT 13:57:52 ON 22 APR 2004
L46          11 S L44
L47           2 S L46 AND L25-L27
L48           9 S L46 NOT L47

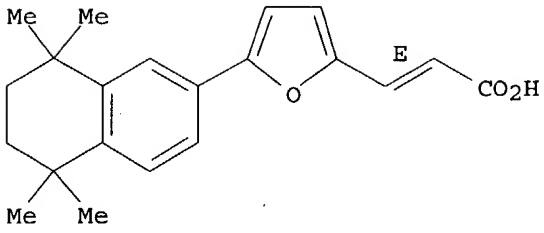
     FILE 'USPATFULL, USPAT2' ENTERED AT 13:58:20 ON 22 APR 2004
L49           9 S L46

     FILE 'REGISTRY' ENTERED AT 13:58:43 ON 22 APR 2004

=> d ide can tot l44

L44  ANSWER 1 OF 36  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   675579-71-2  REGISTRY
CN   2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-
     naphthalenyl)-2-furanyl]-, (2E)- (9CI)  (CA INDEX NAME)
FS   STEREOSEARCH
MF   C21 H24 O3
SR   CA
LC   STN Files:   CAPLUS

Double bond geometry as shown.
```

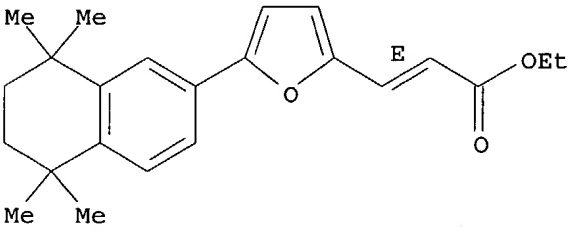


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L44 ANSWER 2 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 675579-70-1 REGISTRY
CN 2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-furanyl]-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C23 H28 O3**
SR CA
LC STN Files: CAPLUS

Double bond geometry as shown.

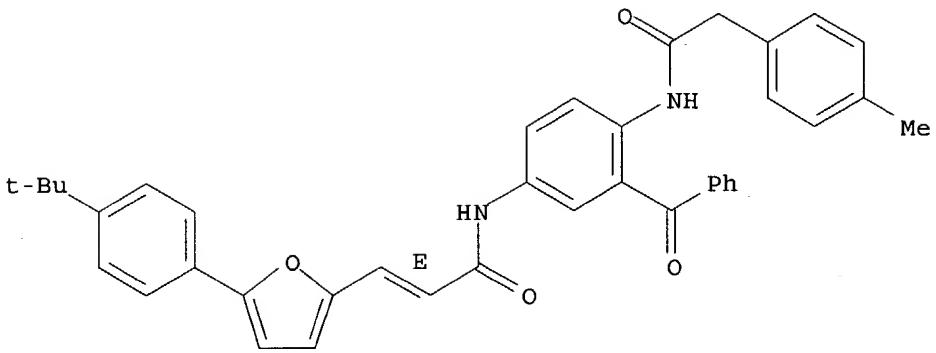


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L44 ANSWER 3 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 493037-21-1 REGISTRY
CN Benzeneacetamide, N-[2-benzoyl-4-[[(2E)-3-[5-[4-(1,1-dimethylethyl)phenyl]-2-furanyl]-1-oxo-2-propenyl]amino]phenyl]-4-methyl- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C39 H36 N2 O4**
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Double bond geometry as shown.



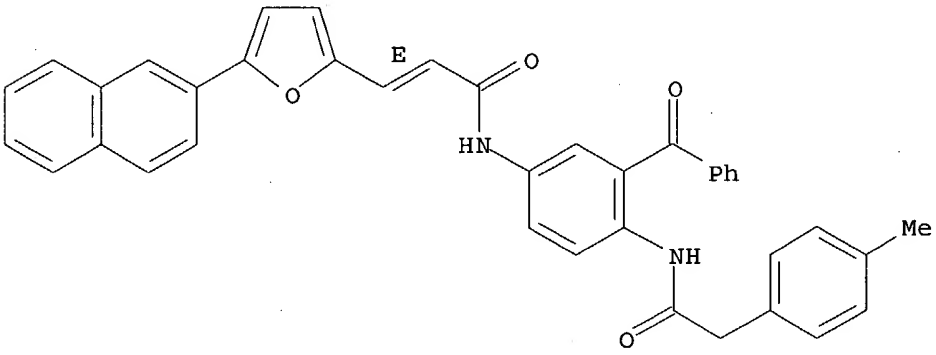
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:137101

L44 ANSWER 4 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 493037-17-5 REGISTRY
CN Benzeneacetamide, N-[2-benzoyl-4-[[(2E)-3-[5-(2-naphthalenyl)-2-furanyl]-1-oxo-2-propenyl]amino]phenyl]-4-methyl- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C39 H30 N2 O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Double bond geometry as shown.



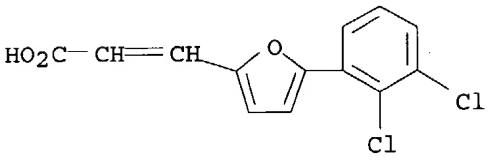
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:137101

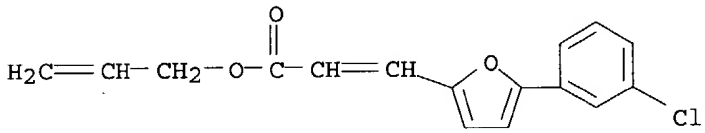
L44 ANSWER 5 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 463351-44-2 REGISTRY
CN 2-Propenoic acid, 3-[5-(2,3-dichlorophenyl)-2-furanyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD

MF **C13 H8 Cl2 O3**
SR Chemical Library
LC STN Files: CHEMCATS



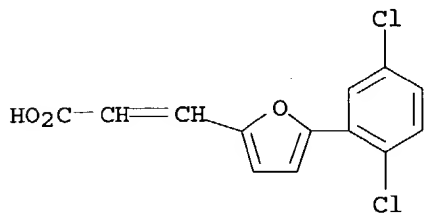
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L44 ANSWER 6 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 372155-49-2 REGISTRY
CN 2-Propenoic acid, 3-[5-(3-chlorophenyl)-2-furanyl]-, 2-propenyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C16 H13 Cl O3**
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

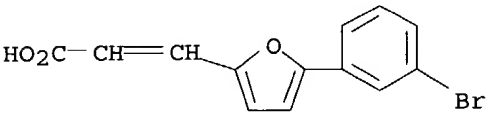
L44 ANSWER 7 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 329795-33-7 REGISTRY
CN 2-Propenoic acid, 3-[5-(2,5-dichlorophenyl)-2-furanyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C13 H8 Cl2 O3**
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L44 ANSWER 8 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN

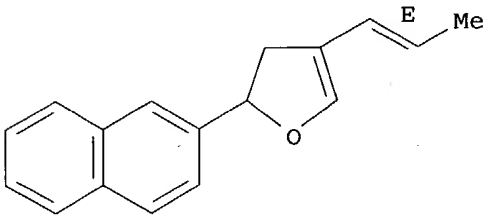
RN 301654-93-3 REGISTRY
CN 2-Propenoic acid, 3-[5-(3-bromophenyl)-2-furanyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C13 H9 Br O3**
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L44 ANSWER 9 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 285565-66-4 REGISTRY
CN Furan, 2,3-dihydro-2-(2-naphthalenyl)-4-(1E)-1-propenyl- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C17 H16 O
SR CA
LC STN Files: CA, CAPLUS

Double bond geometry as shown.



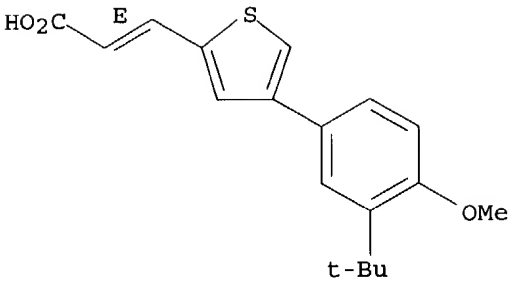
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 133:135199

L44 ANSWER 10 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 241140-33-0 REGISTRY
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C18 H20 O3 S**
SR CA
LC STN Files: CA, CAPLUS

Double bond geometry as shown.



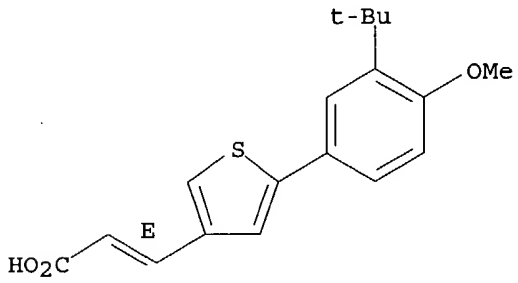
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:194472

L44 ANSWER 11 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 241140-32-9 REGISTRY
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]-, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C18 H20 O3 S**
SR CA
LC STN Files: CA, CAPLUS

Double bond geometry as shown.



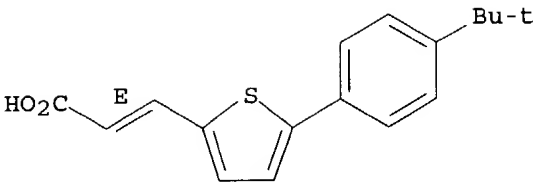
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:194472

L44 ANSWER 12 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 229008-57-5 REGISTRY
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C17 H18 O2 S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

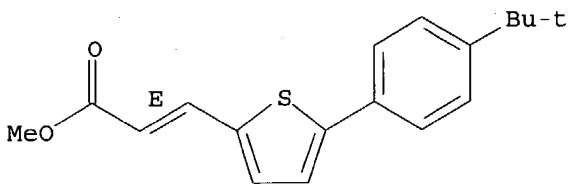
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:87834

REFERENCE 2: 131:73571

L44 ANSWER 13 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 229008-56-4 REGISTRY
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C18 H20 O2 S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

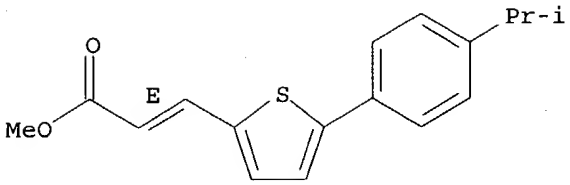
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:87834

REFERENCE 2: 131:73571

L44 ANSWER 14 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 229008-54-2 REGISTRY
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C17 H18 O2 S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

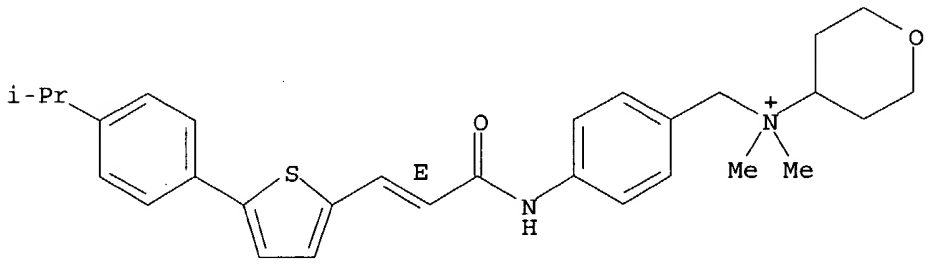
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:87834

REFERENCE 2: 131:73571

L44 ANSWER 15 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 229006-12-6 REGISTRY
CN 2H-Pyran-4-aminium, tetrahydro-N,N-dimethyl-N-[[4-[[(2E)-3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-1-oxo-2-propenyl]amino]phenyl]methyl]-, iodide (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C30 H37 N2 O2 S . I**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.



● I⁻

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

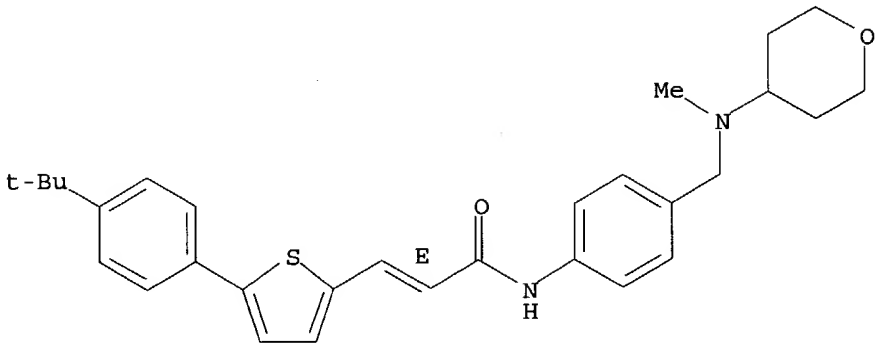
REFERENCE 1: 131:87834

REFERENCE 2: 131:73571

L44 ANSWER 16 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 229006-08-0 REGISTRY
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C30 H36 N2 O2 S**
SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

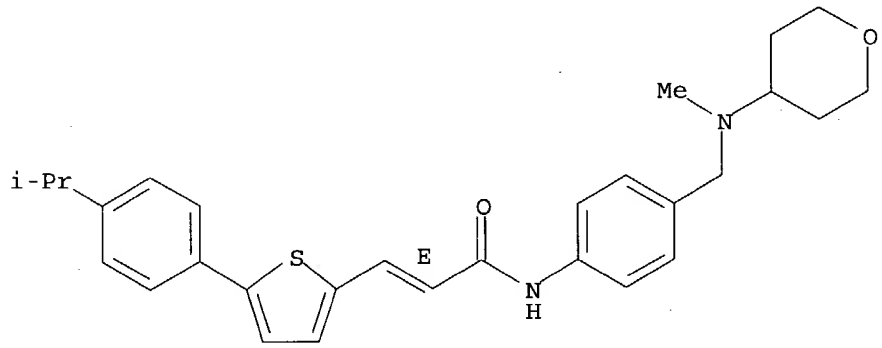
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:87834

REFERENCE 2: 131:73571

L44 ANSWER 17 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 229006-06-8 REGISTRY
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C29 H34 N2 O2 S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

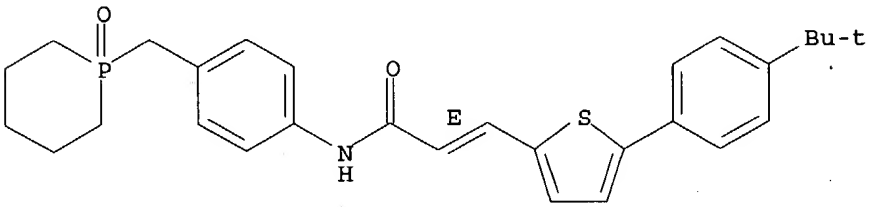
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:87834

REFERENCE 2: 131:73571

L44 ANSWER 18 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 229006-02-4 REGISTRY
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C29 H34 N O2 P S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.



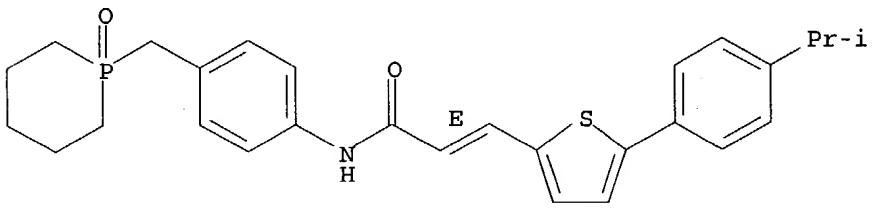
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:87834

REFERENCE 2: 131:73571

L44 ANSWER 19 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 229006-01-3 REGISTRY
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C28 H32 N O2 P S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.



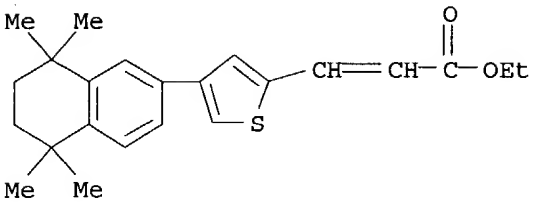
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:87834

REFERENCE 2: 131:73571

L44 ANSWER 20 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN **196961-08-7** REGISTRY
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C23 H28 O2 S**

SR CA
LC STN Files: CA, CAPLUS, USPATFULL

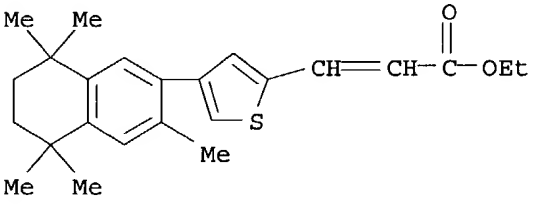


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:293119

L44 ANSWER 21 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN **196961-06-5** REGISTRY
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C24 H30 O2 S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

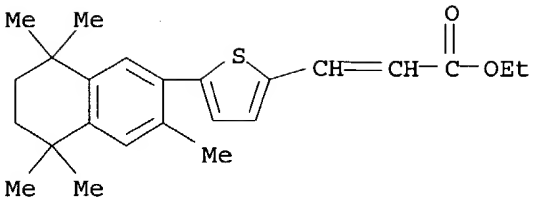


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:293119

L44 ANSWER 22 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN **196961-04-3** REGISTRY
CN 2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C24 H30 O2 S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

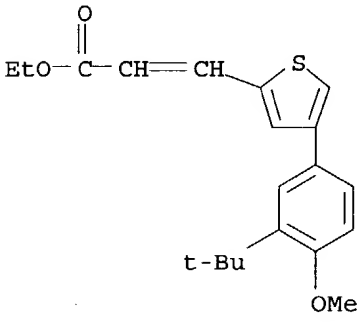


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:293119

L44 ANSWER 23 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN **196961-02-1** REGISTRY
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C20 H24 O3 S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

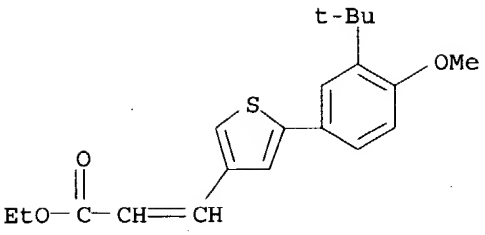


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:293119

L44 ANSWER 24 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN **196961-00-9** REGISTRY
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C20 H24 O3 S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

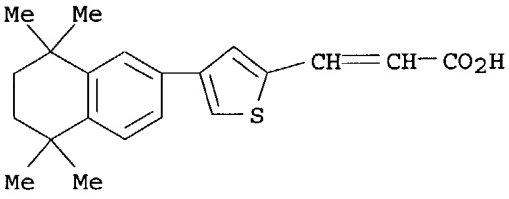


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:293119

L44 ANSWER 25 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN **196960-65-3** REGISTRY
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C21 H24 O2 S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

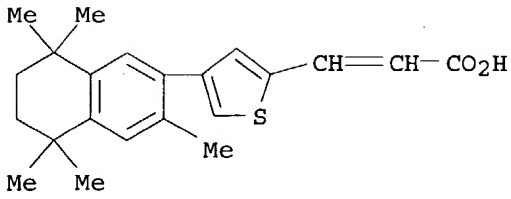


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:293119

L44 ANSWER 26 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN **196960-64-2** REGISTRY
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C22 H26 O2 S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

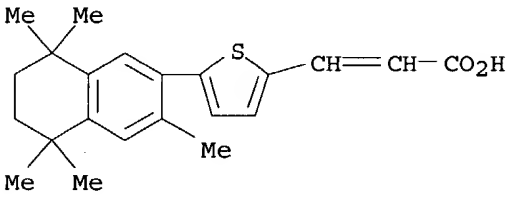


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:293119

L44 ANSWER 27 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN **196960-63-1** REGISTRY
CN 2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C22 H26 O2 S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

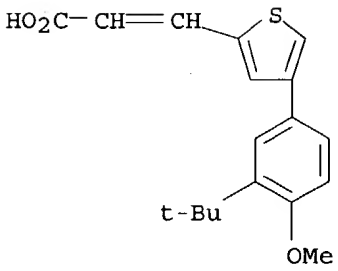


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:293119

L44 ANSWER 28 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN **196960-62-0** REGISTRY
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C18 H20 O3 S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

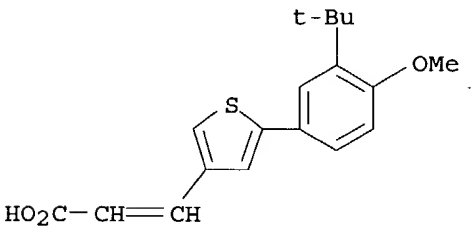


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:293119

L44 ANSWER 29 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN **196960-61-9** REGISTRY
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C18 H20 O3 S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

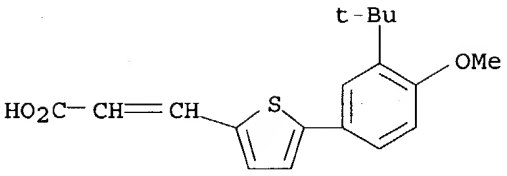


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:293119

L44 ANSWER 30 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN **196960-59-5** REGISTRY
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C18 H20 O3 S**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



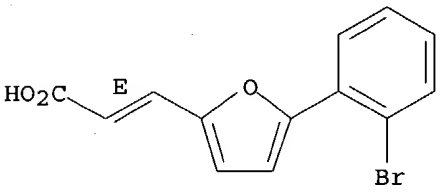
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:293119

L44 ANSWER 31 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 129626-52-4 REGISTRY
CN 2-Propenoic acid, 3-[5-(2-bromophenyl)-2-furanyl]-, (E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C13 H9 Br O3**
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CHEMCATS
(*File contains numerically searchable property data)

Double bond geometry as shown.



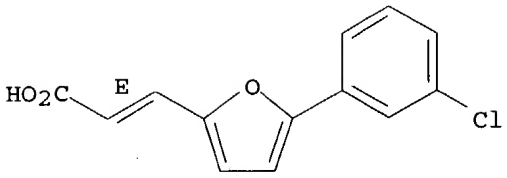
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 113:152173

L44 ANSWER 32 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 62806-36-4 REGISTRY
CN 2-Propenoic acid, 3-[5-(3-chlorophenyl)-2-furanyl]-, (E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C13 H9 Cl O3**
LC STN Files: BEILSTEIN*, CA, CAPLUS, CHEMCATS
(*File contains numerically searchable property data)

Double bond geometry as shown.

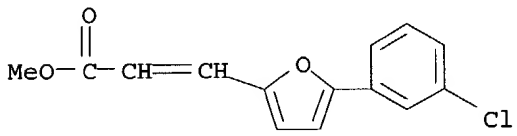


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 86:188948

L44 ANSWER 33 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 58110-51-3 REGISTRY
CN 2-Propenoic acid, 3-[5-(3-chlorophenyl)-2-furanyl]-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C14 H11 Cl O3**
LC STN Files: CA, CAPLUS

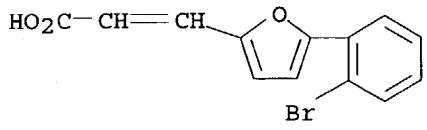


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 84:58390

L44 ANSWER 34 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 58110-41-1 REGISTRY
CN 2-Propenoic acid, 3-[5-(2-bromophenyl)-2-furanyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C13 H9 Br O3**
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS
(*File contains numerically searchable property data)



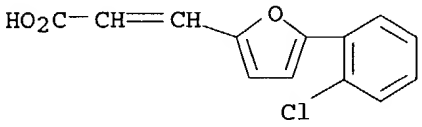
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 109:110184

REFERENCE 2: 84:58390

L44 ANSWER 35 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 58110-39-7 REGISTRY
CN 2-Propenoic acid, 3-[5-(2-chlorophenyl)-2-furanyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C13 H9 Cl O3**
LC STN Files: CA, CAPLUS, CHEMCATS

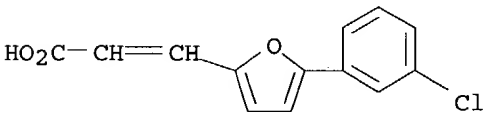


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 84:58390

L44 ANSWER 36 OF 36 REGISTRY COPYRIGHT 2004 ACS on STN
RN 58110-38-6 REGISTRY
CN 2-Propenoic acid, 3-[5-(3-chlorophenyl)-2-furanyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C13 H9 Cl O3**
LC STN Files: BEILSTEIN*, CA, CAPLUS, CHEMCATS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 84:58390

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CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 13:59:02 ON 22 APR 2004
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

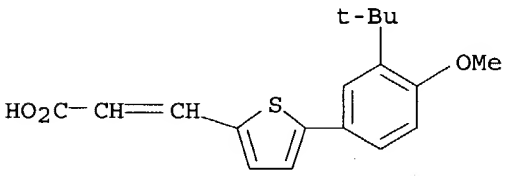
=> d bib abs hitstr tot l49

L49 ANSWER 1 OF 9 USPATFULL on STN
AN 2003:195242 USPATFULL
TI Bicyclic aromatic compounds

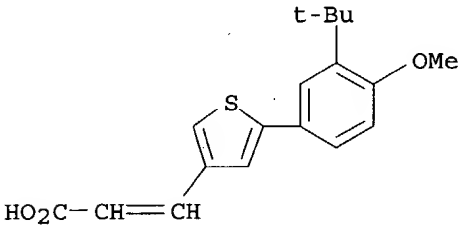
IN Bernardon, Jean-Michel, Le Rouret, FRANCE
PI US 2003135053 A1 20030717
AI US 2003-334978 A1 20030102 (10)
RLI Continuation of Ser. No. US 2000-619584, filed on 19 Jul 2000, PENDING Division of Ser. No. US 1998-952804, filed on 26 Jan 1998, GRANTED, Pat. No. US 6147255 A 371 of International Ser. No. WO 1997-FR391, filed on 5 Mar 1997, UNKNOWN
PRAI FR 1996-3235 19960314
DT Utility
FS APPLICATION
LREP BURNS, DOANE, SWECKER & MATHIS, L.L.P., P.O. Box 1404, Alexandria, VA, 22313-1404
CLMN Number of Claims: 11
ECL Exemplary Claim: 1
DRWN 1 Drawing Page(s)
LN.CNT 1588
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The invention relates to novel bicyclic aromatic compounds which have the general formula (I): ##STR1##

as well as to the use of these compounds in pharmaceutical compositions intended for use in human or veterinary medicine (dermatological, rheumatic, respiratory, cardiovascular and ophthalmological complaints in particular), or alternatively in cosmetic compositions.

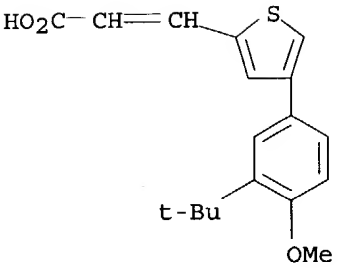
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **196960-59-5P 196960-61-9P 196960-62-0P 196960-63-1P 196960-64-2P 196960-65-3P**
(preparation of bicyclic aromatic compds.)
RN 196960-59-5 USPATFULL
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]- (9CI) (CA INDEX NAME)



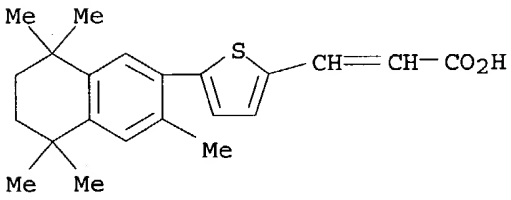
RN 196960-61-9 USPATFULL
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]- (9CI) (CA INDEX NAME)



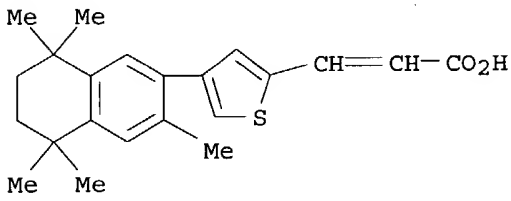
RN 196960-62-0 USPATFULL
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]- (9CI) (CA INDEX NAME)



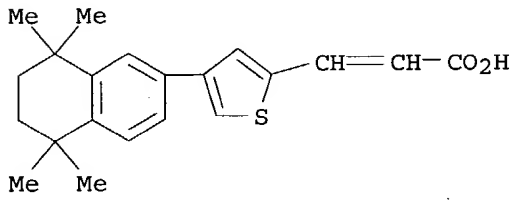
RN 196960-63-1 USPATFULL
CN 2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)



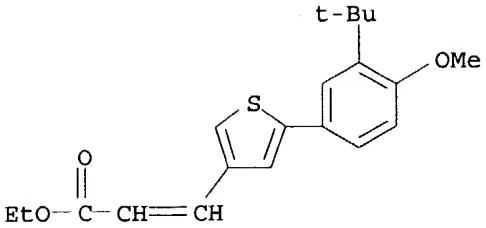
RN 196960-64-2 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)



RN 196960-65-3 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)



IT **196961-00-9P 196961-02-1P 196961-04-3P**
196961-06-5P 196961-08-7P
(preparation of bicyclic aromatic compds.)
RN 196961-00-9 USPATFULL
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 196961-02-1 USPATFULL
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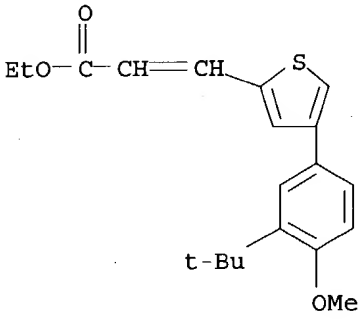
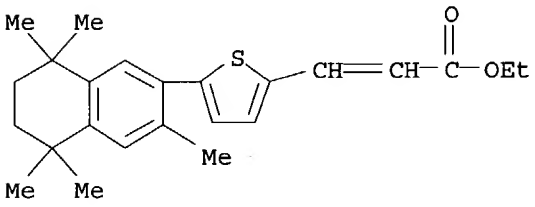
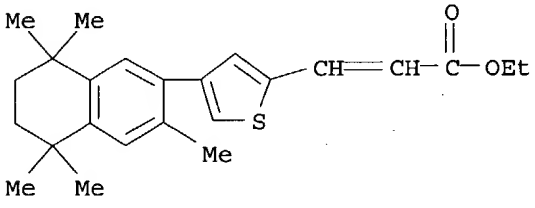


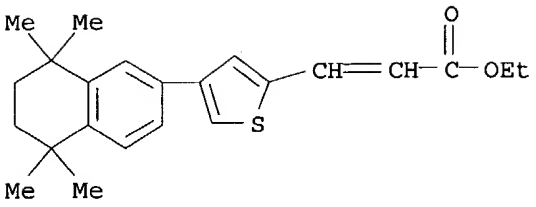
RN 196961-04-3 USPATFULL
CN 2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 196961-06-5 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



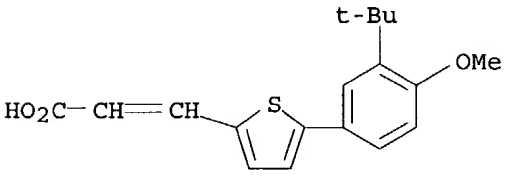
RN 196961-08-7 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



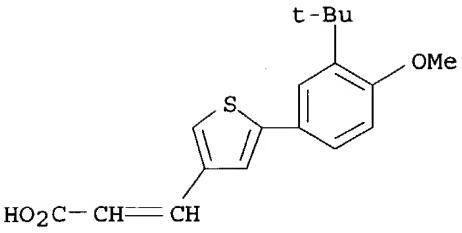
L49 ANSWER 2 OF 9 USPATFULL on STN
AN 2003:86883 USPATFULL
TI Bicyclic aromatic compounds
IN Bernardon, Jean-Michel, Le Rouret, FRANCE
PI US 2003060491 A1 20030327
AI US 2002-252514 A1 20020924 (10)
RLI Division of Ser. No. US 2000-619582, filed on 19 Jul 2000, PENDING
Continuation of Ser. No. US 1998-952804, filed on 26 Jan 1998, GRANTED, Pat. No. US 6147255 A 371 of International Ser. No. WO 1997-FR391, filed on 5 Mar 1997, UNKNOWN
PRAI FR 1996-3235 19960314
DT Utility
FS APPLICATION
LREP Norman H. Stepno, BURNS, DOANE, SWECKER & MATHIS, L.L.P., P.O. Box1404, Alexandria, VA, 22313-1404
CLMN Number of Claims: 11
ECL Exemplary Claim: 1
DRWN 1 Drawing Page(s)
LN.CNT 1584
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The invention relates to novel bicyclic aromatic compounds which have the general formula (I): ##STR1##

as well as to the use of these compounds in pharmaceutical compositions intended for use in human or veterinary medicine (dermatological, rheumatic, respiratory, cardiovascular and ophthalmological complaints in particular), or alternatively in cosmetic compositions.

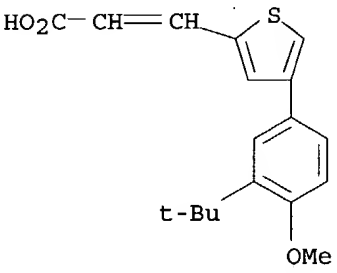
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **196960-59-5P 196960-61-9P 196960-62-0P**
196960-63-1P 196960-64-2P 196960-65-3P
(preparation of bicyclic aromatic compds.)
RN 196960-59-5 USPATFULL
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]- (9CI) (CA INDEX NAME)



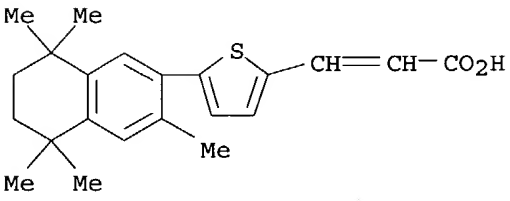
RN 196960-61-9 USPATFULL
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]- (9CI) (CA INDEX NAME)



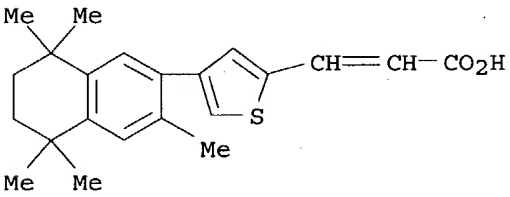
RN 196960-62-0 USPATFULL
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]- (9CI) (CA INDEX NAME)



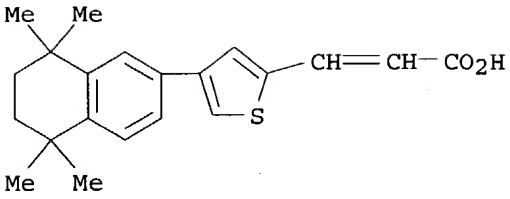
RN 196960-63-1 USPATFULL
CN 2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)



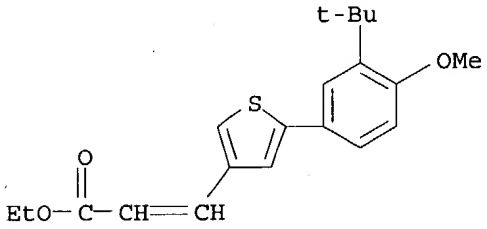
RN 196960-64-2 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)



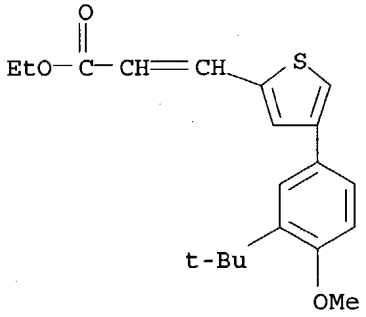
RN 196960-65-3 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)



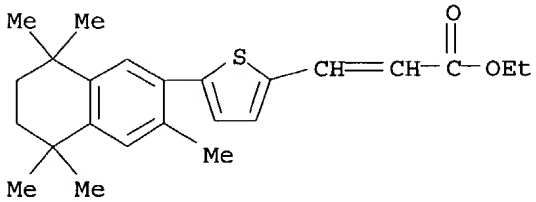
IT **196961-00-9P 196961-02-1P 196961-04-3P**
196961-06-5P 196961-08-7P
(preparation of bicyclic aromatic compds.)
RN 196961-00-9 USPATFULL
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



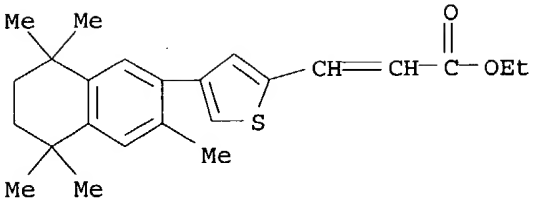
RN 196961-02-1 USPATFULL
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



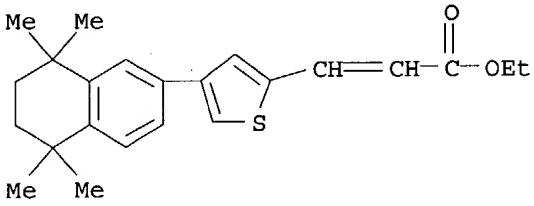
RN 196961-04-3 USPATFULL
CN 2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 196961-06-5 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



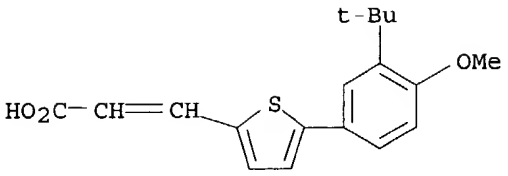
RN 196961-08-7 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



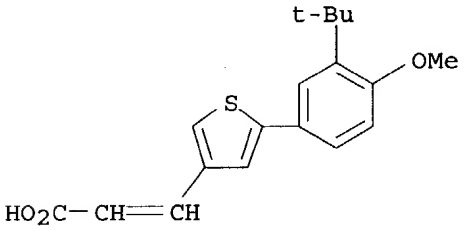
L49 ANSWER 3 OF 9 USPATFULL on STN
AN 2003:33507 USPATFULL
TI Bicyclic aromatic compounds
IN Bernardon, Jean-Michel, Le Rouret, FRANCE
PA Centre International de Recherches Dermatologiques Galderma, Valbonne, FRANCE (non-U.S. corporation)
PI US 6515021 B1 20030204
AI US 2000-619582 20000912 (9)
RLI Continuation of Ser. No. US 952804, now patented, Pat. No. US 6147255
PRAI FR 1996-3235 19960314
DT Utility
FS GRANTED
EXNAM Primary Examiner: Qazi, Sabiha
LREP Burns, Doane, Swecker & Mathis, L.L.P.
CLMN Number of Claims: 9
ECL Exemplary Claim: 1
DRWN 2 Drawing Figure(s); 1 Drawing Page(s)
LN.CNT 1480
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The invention relates to novel bicyclic aromatic compounds which have the general formula (I): ##STR1##

as well as to the use of these compounds in pharmaceutical compositions intended for use in human or veterinary medicine (dermatological, rheumatic, respiratory, cardiovascular and ophthalmological complaints in particular), or alternatively in cosmetic compositions.

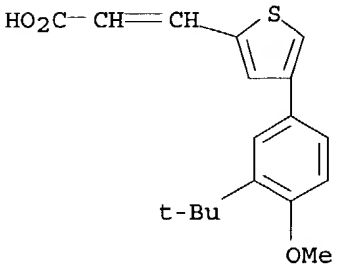
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **196960-59-5P 196960-61-9P 196960-62-0P 196960-63-1P 196960-64-2P 196960-65-3P**
(preparation of bicyclic aromatic compds.)
RN 196960-59-5 USPATFULL
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]- (9CI) (CA INDEX NAME)



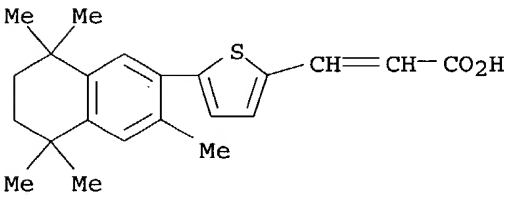
RN 196960-61-9 USPATFULL
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]- (9CI) (CA INDEX NAME)



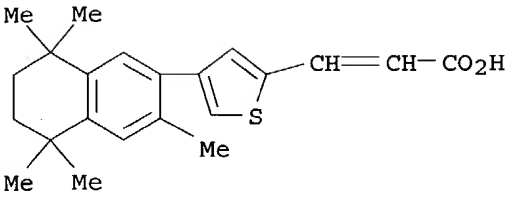
RN 196960-62-0 USPATFULL
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]- (9CI) (CA INDEX NAME)



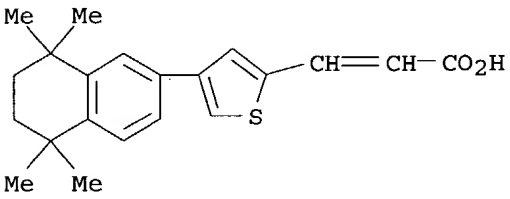
RN 196960-63-1 USPATFULL
CN 2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)



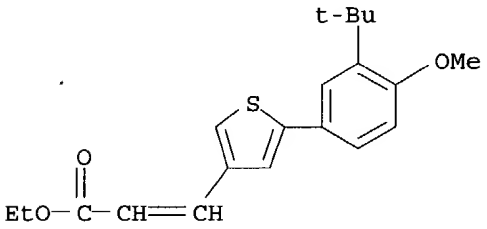
RN 196960-64-2 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)



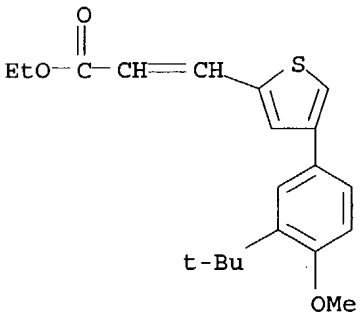
RN 196960-65-3 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)



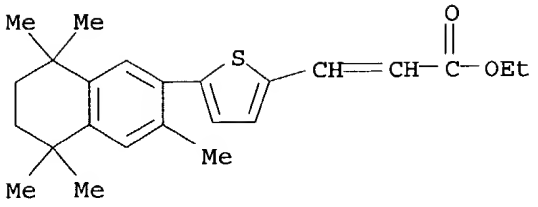
IT **196961-00-9P 196961-02-1P 196961-04-3P 196961-06-5P 196961-08-7P**
(preparation of bicyclic aromatic compds.)
RN 196961-00-9 USPATFULL
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



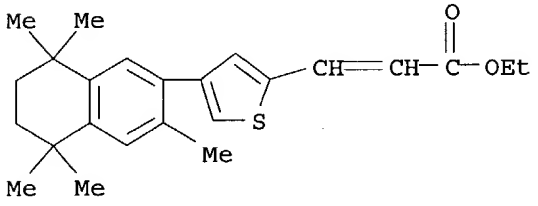
RN 196961-02-1 USPATFULL
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



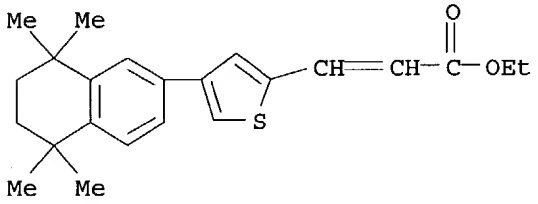
RN 196961-04-3 USPATFULL
CN 2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 196961-06-5 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 196961-08-7 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



L49 ANSWER 4 OF 9 USPATFULL on STN
AN 2002:160710 USPATFULL
TI Anilide derivative, production and use thereof
IN Shiraishi, Mitsuru, Hyogo, JAPAN
Kitayoshi, Takahito, Osaka, JAPAN
Aramaki, Yoshio, Hyogo, JAPAN
Honda, Susumu, Hyogo, JAPAN
Oda, Tsuneo, Osaka, JAPAN
PA Takeda Chemical Industries, Ltd., Osaka, JAPAN (non-U.S. corporation)
PI US 6413947 B1 20020702
AI US 2000-661194 20000913 (9)
RLI Division of Ser. No. US 1998-213379, filed on 17 Dec 1998, now patented, Pat. No. US 6166006
PRAI JP 1997-351481 19971219
DT Utility
FS GRANTED
EXNAM Primary Examiner: Powers, Fiona T.
LREP Wenderoth, Lind & Ponack, L.L.P.
CLMN Number of Claims: 18
ECL Exemplary Claim: 1
DRWN 0 Drawing Figure(s); 0 Drawing Page(s)
LN.CNT 15864
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention is to provide a compound of the formula: ##STR1##

wherein R.sup.1 is an optionally substituted 5- to 6-membered ring; W is a divalent group of the formula: ##STR2##

wherein the ring A is an optionally substituted 5- to 6-membered aromatic ring, X is an optionally substituted C, N or O atom, and the ring B is an optionally substituted 5- to 7-membered ring; Z is a chemical bond or a divalent group; R.sup.2 is (1) an, optionally substituted amino group in which a nitrogen atom may form a quaternary ammonium, etc., or a salt thereof, which is useful for antagonizing MCP-1 receptor.

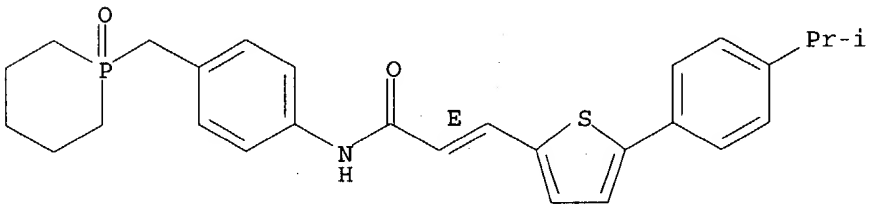
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **229006-01-3P 229006-02-4P 229006-06-8P**
229006-08-0P 229006-12-6P
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

RN 229006-01-3 USPATFULL

CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

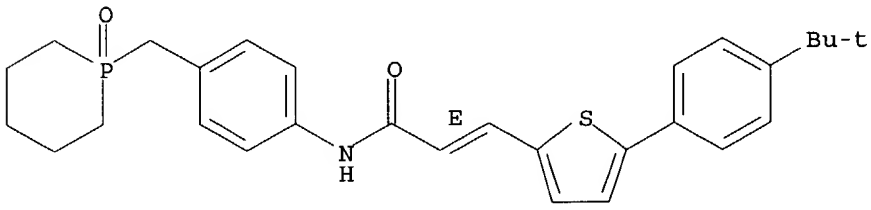
Double bond geometry as shown.



RN 229006-02-4 USPATFULL

CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

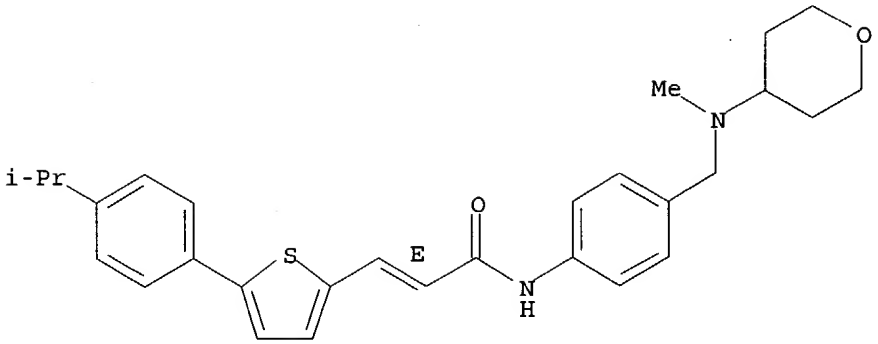
Double bond geometry as shown.



RN 229006-06-8 USPATFULL

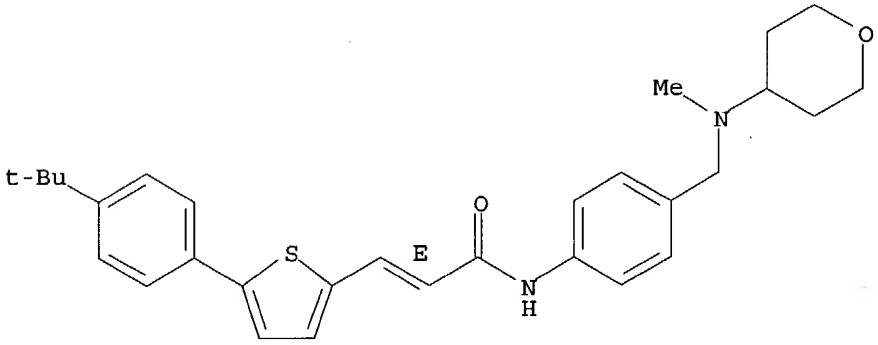
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



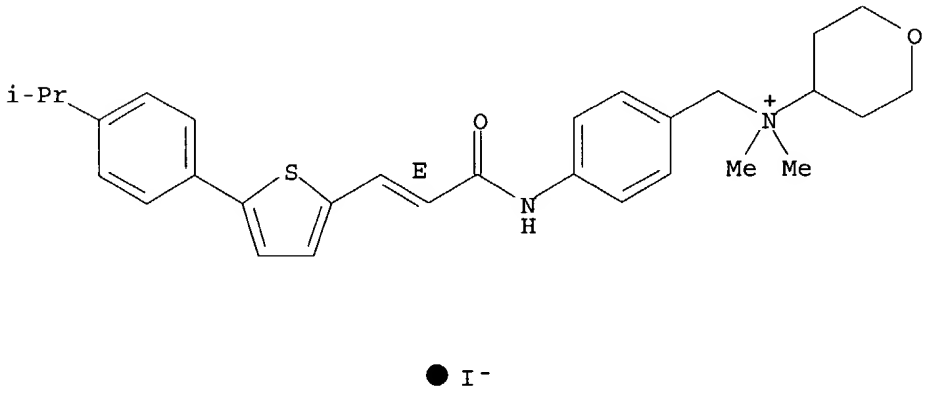
RN 229006-08-0 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229006-12-6 USPATFULL
CN 2H-Pyran-4-aminium, tetrahydro-N,N-dimethyl-N-[[4-[[(2E)-3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-1-oxo-2-propenyl]amino]phenyl]methyl]-, iodide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

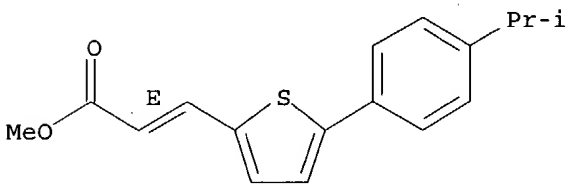


● I⁻

IT **229008-54-2P 229008-56-4P 229008-57-5P**
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

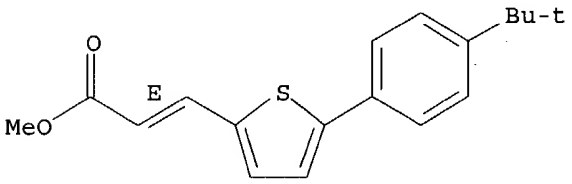
RN 229008-54-2 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



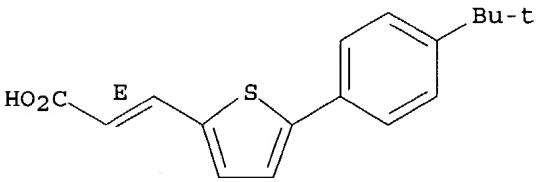
RN 229008-56-4 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229008-57-5 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



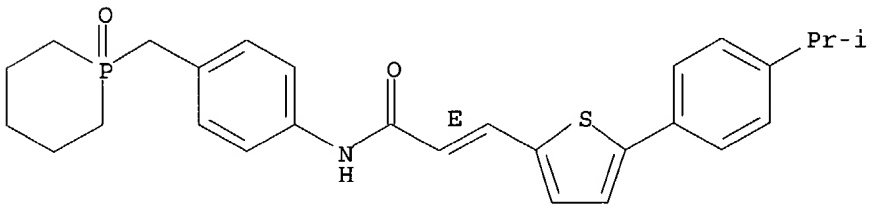
L49 ANSWER 5 OF 9 USPATFULL on STN
AN 2002:88517 USPATFULL
TI Quaternary ammonium salts and their use
IN Shiraishi, Mitsuru, Hyogo, JAPAN
Baba, Masanori, Kagoshima, JAPAN
Aramaki, Yoshio, Hyogo, JAPAN
Nishimura, Osamu, Ibaraki, JAPAN
Kanzaki, Naoyuki, Osaka, JAPAN
PA Takeda Chemical Industries, Ltd., Osaka, JAPAN (non-U.S. corporation)
PI US 6376536 B1 20020423
AI US 2000-580270 20000526 (9)
RLI Division of Ser. No. US 1999-377040, filed on 19 Aug 1999, now patented, Pat. No. US 6096780
PRAI JP 1998-234388 19980820
US 1998-104845P 19981016 (60)
DT Utility
FS GRANTED

EXNAM Primary Examiner: Solola, T. A.
LREP Wenderoth, Lind & Ponack, L.L.P.
CLMN Number of Claims: 7
ECL Exemplary Claim: 1
DRWN 0 Drawing Figure(s); 0 Drawing Page(s)
LN.CNT 2156
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB This invention is to provide a compound for antagonizing CCR5, said compound being represented by the formula: ##STR1##

wherein R.sup.1 is an optionally substituted phenyl or an optionally substituted thienyl; Y is --CH.sub.2--, --S-- or --O--; and R.sup.2, R.sup.3 and R.sup.4 are independently an optionally substituted aliphatic hydrocarbon group or an optionally substituted alicyclic heterocyclic ring group, and being effective for the prevention and treatment of infectious disease of HIV.

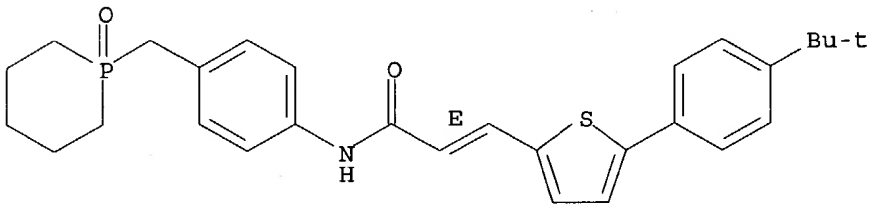
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **229006-01-3P 229006-02-4P 229006-06-8P**
229006-08-0P 229006-12-6P
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)
RN 229006-01-3 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



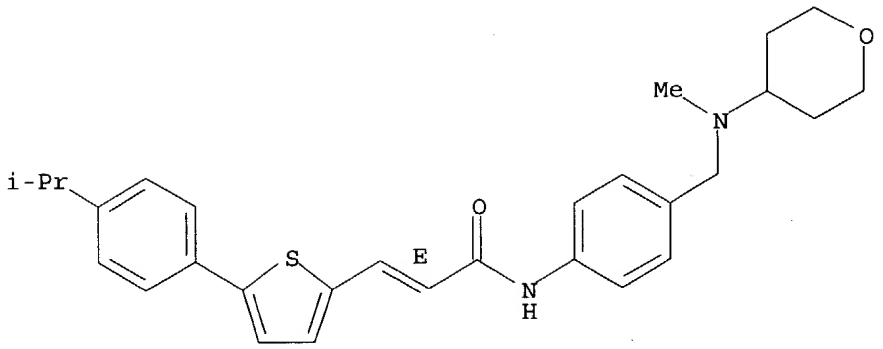
RN 229006-02-4 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



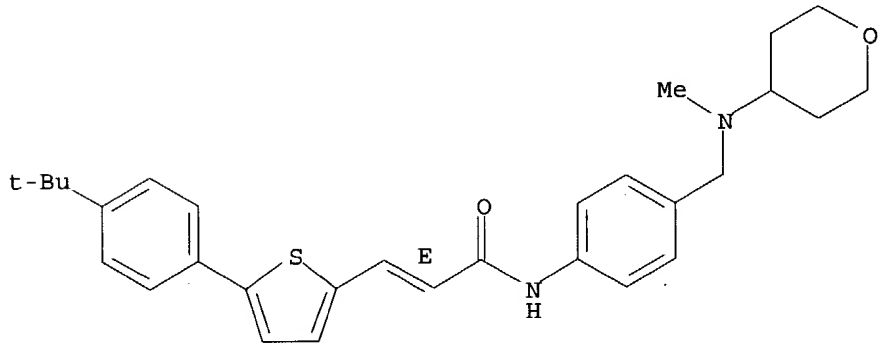
RN 229006-06-8 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



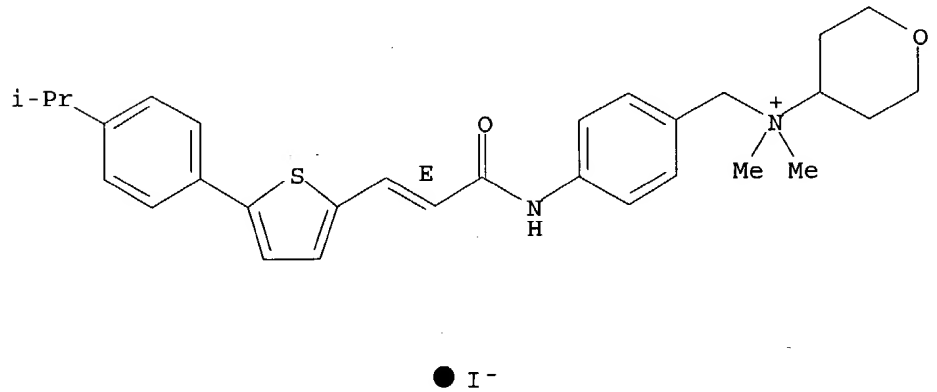
RN 229006-08-0 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229006-12-6 USPATFULL
CN 2H-Pyran-4-aminium, tetrahydro-N,N-dimethyl-N-[[4-[[(2E)-3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-1-oxo-2-propenyl]amino]phenyl]methyl]-, iodide (9CI) (CA INDEX NAME)

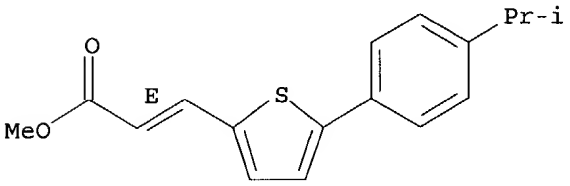
Double bond geometry as shown.



IT **229008-54-2P 229008-56-4P 229008-57-5P**
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

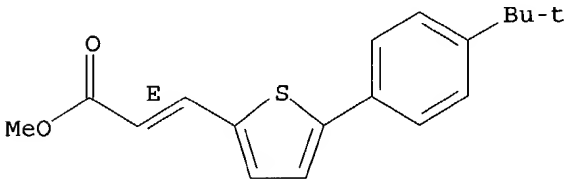
RN 229008-54-2 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



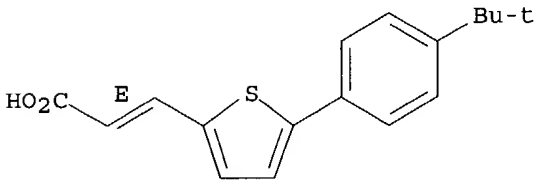
RN 229008-56-4 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229008-57-5 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L49 ANSWER 6 OF 9 USPATFULL on STN
AN 2001:121461 USPATFULL
TI Pharmaceutical composition for antagonizing CCR5 comprising anilide derivative
IN Nishimura, Osamu, Hyogo, Japan
Baba, Masanori, Kagoshima, Japan
Sawada, Hidekazu, Osaka, Japan
Kanzaki, Naoyuki, Osaka, Japan
Kuroshima, Ken-ichi, Osaka, Japan
Shiraishi, Mitsuru, Hyogo, Japan
Aramaki, Yoshio, Hyogo, Japan
PA Takeda Chemical Industries, Ltd., Osaka, Japan (non-U.S. corporation)
PI US 6268354 B1 20010731
AI US 2000-661320 20000913 (9)
RLI Division of Ser. No. US 1998-213377, filed on 17 Dec 1998, now patented, Pat. No. US 6172061
PRAI JP 1997-351480 19971219

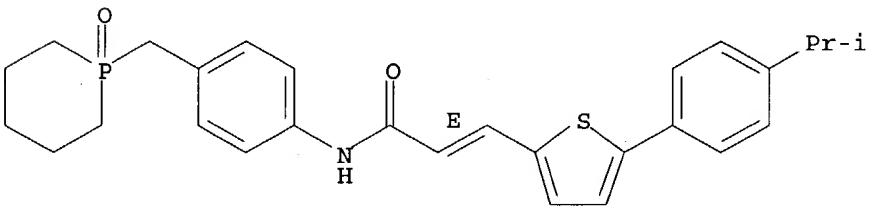
JP 1998-218875 19980803
JP 1998-234388 19980820
US 1998-104847P 19981116 (60)
US 1998-104845P 19981116 (60)
DT Utility
FS GRANTED
EXNAM Primary Examiner: Powers, Fiona T.
LREP Wenderoth, Lind & Ponack, L.L.P.
CLMN Number of Claims: 21
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 16650
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB This invention is to provide a pharmaceutical composition for antagonizing CCR5 which comprises a compound of the formula: ##STR1##

wherein R.sup.1 is an optionally substituted 5- to 6-membered ring; W is a divalent group of the formula: ##STR2##

wherein the ring A is an optionally substituted 5- to 6-membered aromatic ring, X is an optionally substituted C, N or O atom, and the ring B is an optionally substituted 5- to 7-membered ring; Z is a chemical bond or a divalent group; R.sup.2 is (1) an optionally substituted amino group in which a nitrogen atom may form a quaternary ammonium, etc., or a salt thereof.

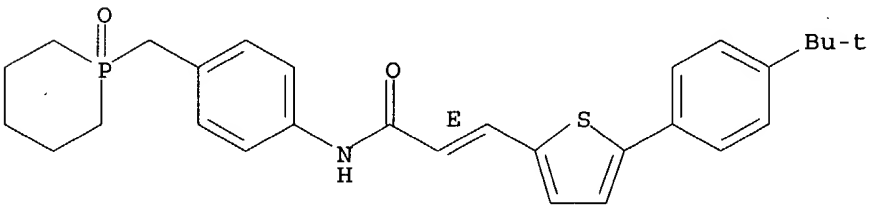
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **229006-01-3P 229006-02-4P 229006-06-8P**
229006-08-0P 229006-12-6P
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)
RN 229006-01-3 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



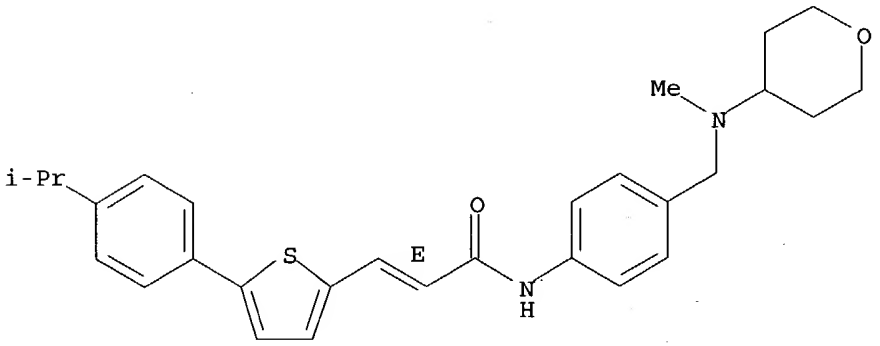
RN 229006-02-4 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



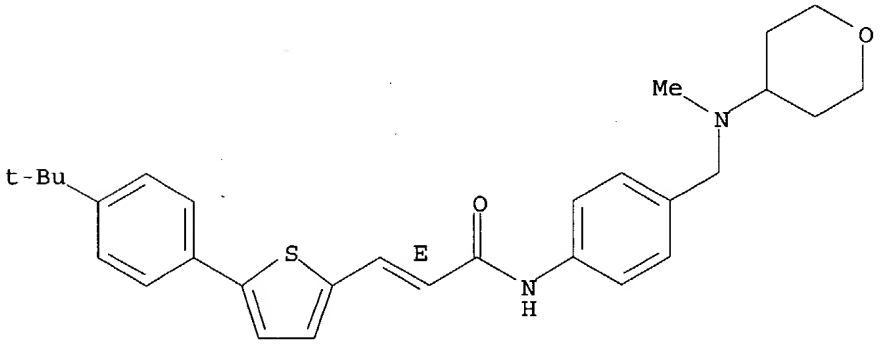
RN 229006-06-8 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



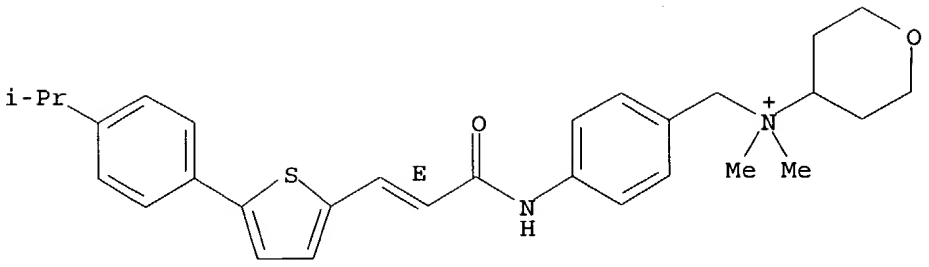
RN 229006-08-0 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229006-12-6 USPATFULL
CN 2H-Pyran-4-aminium, tetrahydro-N,N-dimethyl-N-[[4-[[(2E)-3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-1-oxo-2-propenyl]amino]phenyl]methyl]-, iodide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

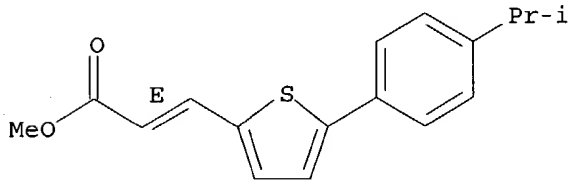


● I^-

IT **229008-54-2P 229008-56-4P 229008-57-5P**
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

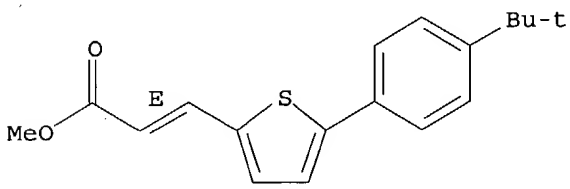
RN 229008-54-2 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



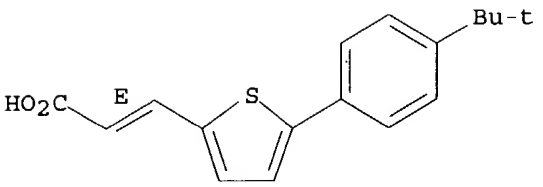
RN 229008-56-4 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229008-57-5 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

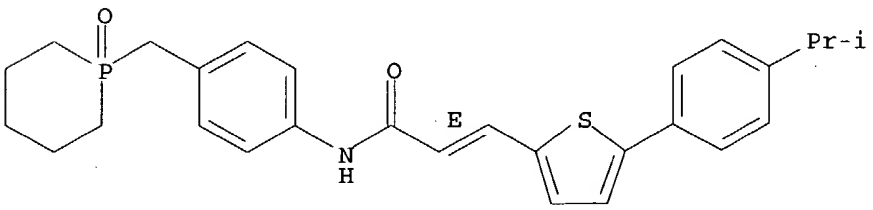
Double bond geometry as shown.



L49 ANSWER 7 OF 9 USPATFULL on STN
AN 2000:174633 USPATFULL
TI Anilide derivative, production and use thereof
IN Shiraishi, Mitsuru, Hyogo, Japan
Kitayoshi, Takahito, Osaka, Japan
Aramaki, Yoshio, Hyogo, Japan
Honda, Susumu, Hyogo, Japan
Oda, Tsuneo, Osaka, Japan
PA Takeda Chemical Industries, Ltd., Osaka, Japan (non-U.S. corporation)
PI US 6166006 20001226
AI US 1998-213379 19981217 (9)
PRAI JP 1997-351481 19971219
DT Utility
FS Granted
EXNAM Primary Examiner: Powers, Fiona T.
LREP Wenderoth, Lind & Ponack, L.L.P.
CLMN Number of Claims: 26
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 15554
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB This invention is to provide a compound of the formula: ##STR1## wherein R.sup.1 is an optionally substituted 5- to 6-membered ring: C is a divalent group of the formula: ##STR2## wherein the ring A is an optionally substituted 5- to 6-membered aromatic ring, X is an optionally substituted C, N or O atom, and the ring B is an optionally substituted 5- to 7-membered ring; Z is a chemical bond or a divalent group; R.sup.2 is (1) an optionally substituted amino group in which a nitrogen atom may form a quaternary ammonium, etc., or a salt thereof, which is useful for antagonizing MCP-1 receptor.

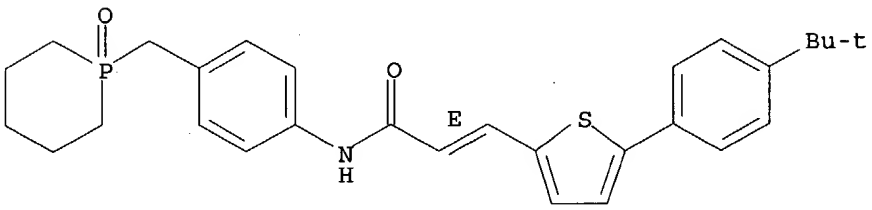
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **229006-01-3P 229006-02-4P 229006-06-8P**
229006-08-0P 229006-12-6P
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)
RN 229006-01-3 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



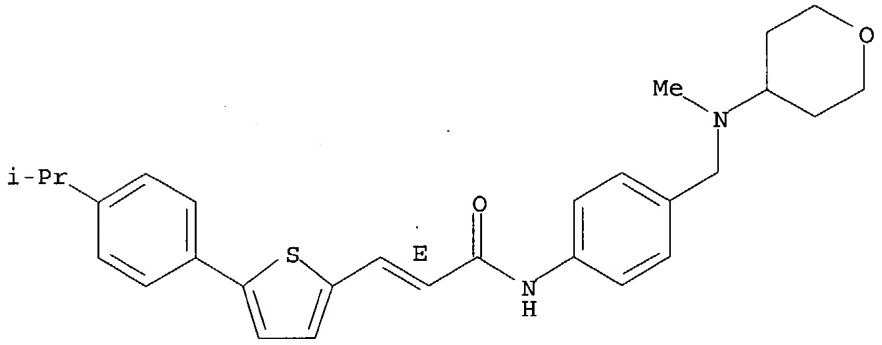
RN 229006-02-4 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



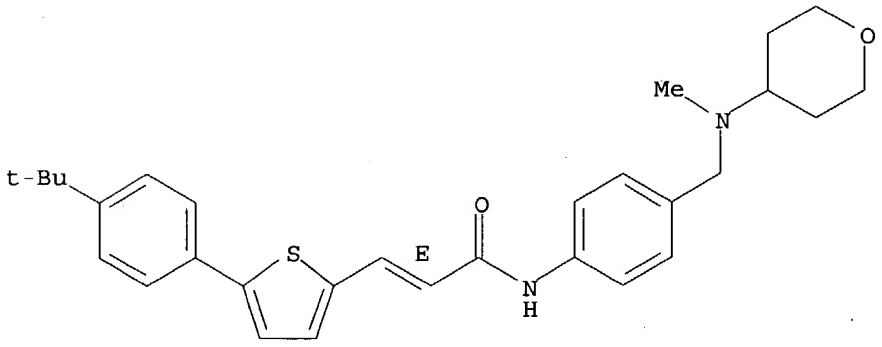
RN 229006-06-8 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



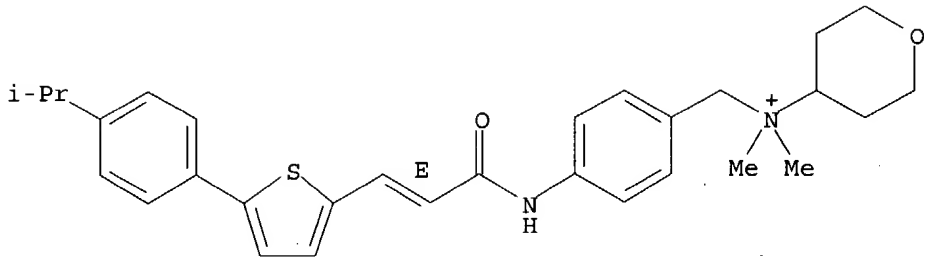
RN 229006-08-0 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229006-12-6 USPATFULL
CN 2H-Pyran-4-aminium, tetrahydro-N,N-dimethyl-N-[[4-[[(2E)-3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-1-oxo-2-propenyl]amino]phenyl]methyl]-, iodide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

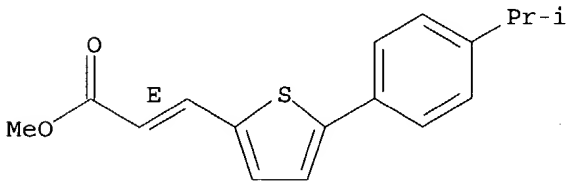


● I^-

IT **229008-54-2P 229008-56-4P 229008-57-5P**
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

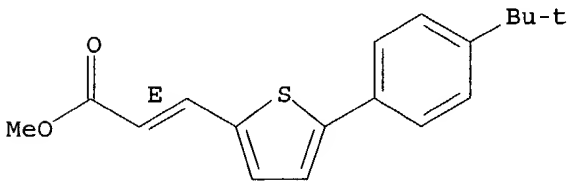
RN 229008-54-2 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



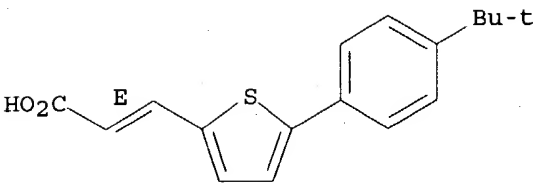
RN 229008-56-4 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



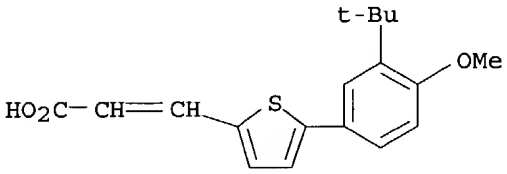
RN 229008-57-5 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

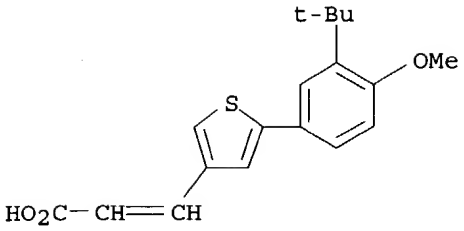


L49 ANSWER 8 OF 9 USPATFULL on STN
AN 2000:153887 USPATFULL
TI Bicyclic-aromatic compounds
IN Bernardon, Jean-Michel, Le Rouret, France
PA Centre International de Recherches Dermatologiques Galderma, Valbonne, France (non-U.S. corporation)
PI US 6147255 20001114
WO 9733881 19970918
AI US 1998-952804 19980126 (8)
WO 1997-FR391 19970305
19980126 PCT 371 date
19980126 PCT 102(e) date
PRAI FR 1996-3235 19960314
DT Utility
FS Granted
EXNAM Primary Examiner: Oazi, Sabiha
LREP Burns, Doane, Swecker & Mathis, L.L.P.
CLMN Number of Claims: 10
ECL Exemplary Claim: 1
DRWN 1 Drawing Figure(s); 1 Drawing Page(s)
LN.CNT 1471
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The invention relates to novel bicyclic aromatic compounds which have the general formula (I): ##STR1## as well as to the use of these compounds in pharmaceutical compositions intended for use in human or veterinary medicine (dermatological, rheumatic, respiratory, cardiovascular and ophthalmological complaints in particular), or alternatively in cosmetic compositions.

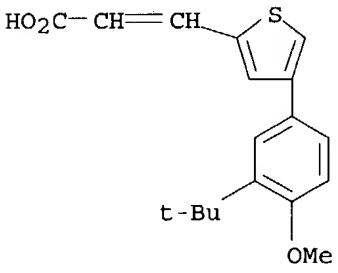
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **196960-59-5P 196960-61-9P 196960-62-0P**
196960-63-1P 196960-64-2P 196960-65-3P
(preparation of bicyclic aromatic compds.)
RN 196960-59-5 USPATFULL
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]- (9CI) (CA INDEX NAME)



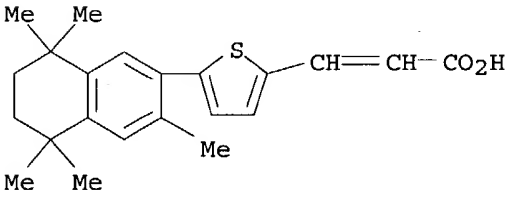
RN 196960-61-9 USPATFULL
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]- (9CI) (CA INDEX NAME)



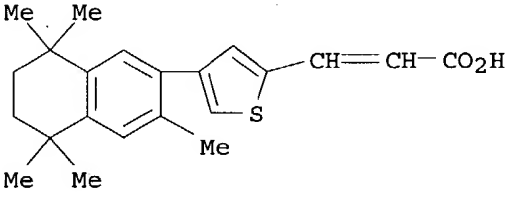
RN 196960-62-0 USPATFULL
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]- (9CI) (CA INDEX NAME)



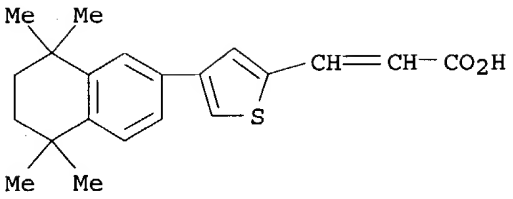
RN 196960-63-1 USPATFULL
CN 2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)



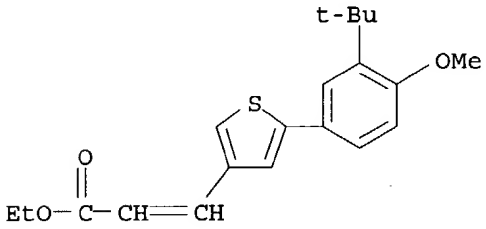
RN 196960-64-2 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)



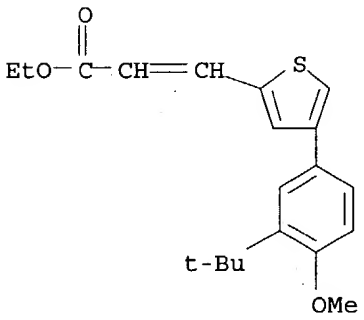
RN 196960-65-3 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)



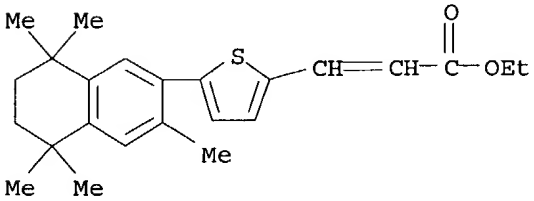
IT **196961-00-9P 196961-02-1P 196961-04-3P**
196961-06-5P 196961-08-7P
(preparation of bicyclic aromatic compds.)
RN 196961-00-9 USPATFULL
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



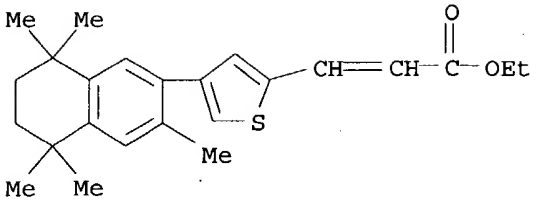
RN 196961-02-1 USPATFULL
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



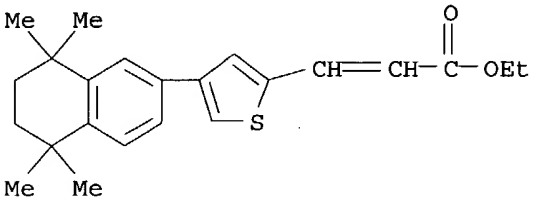
RN 196961-04-3 USPATFULL
CN 2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 196961-06-5 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 196961-08-7 USPATFULL
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)

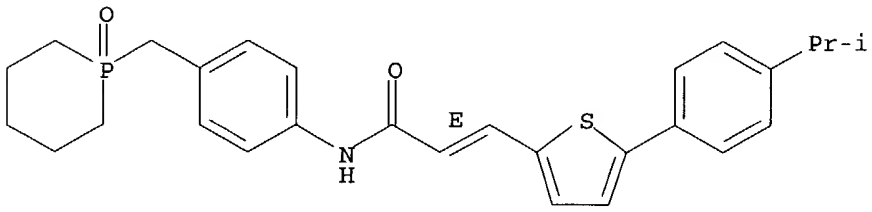


L49 ANSWER 9 OF 9 USPATFULL on STN
AN 2000:98464 USPATFULL
TI Quaternary ammonium salts and their use
IN Shiraishi, Mitsuru, Hyogo, Japan
Baba, Masanori, Kagoshima, Japan
Aramaki, Yoshio, Hyogo, Japan
Nishimura, Osamu, Ibaraki, Japan
Kanzaki, Naoyuki, Osaka, Japan
PA Takeda Chemical Industries, Ltd., Osaka, Japan (non-U.S. corporation)
PI US 6096780 20000801
AI US 1999-377040 19990819 (9)
PRAI JP 1998-234388 19980820
US 1998-104845P 19981016 (60)
DT Utility
FS Granted
EXNAM Primary Examiner: Lambkin, Deborah C.
LREP Wenderoth, Lind & Ponack, LLP.
CLMN Number of Claims: 22
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 2169
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB This invention is to provide a compound for antagonizing CCR5, said compound being represented by the formula: ##STR1## wherein R.sup.1 is an optionally substituted phenyl or an optionally substituted thienyl; Y is --CH.sub.2 --, --S-- or --O--; and R.sup.2, R.sup.3 and R.sup.4 are independently an optionally substituted aliphatic hydrocarbon group or an optionally substituted alicyclic heterocyclic ring group, and being effective for the prevention and treatment of infectious disease of HIV.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **229006-01-3P 229006-02-4P 229006-06-8P**
229006-08-0P 229006-12-6P
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)
RN 229006-01-3 USPATFULL

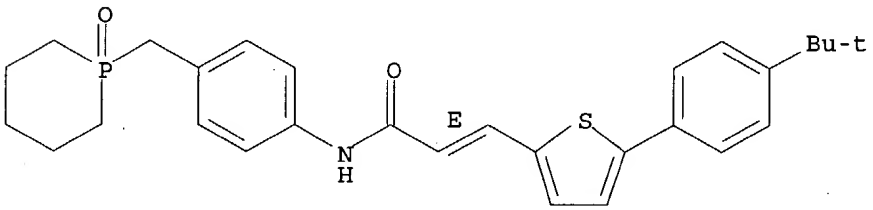
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



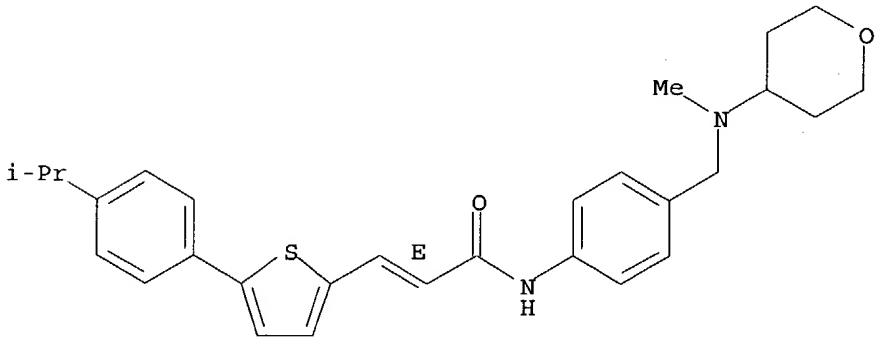
RN 229006-02-4 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



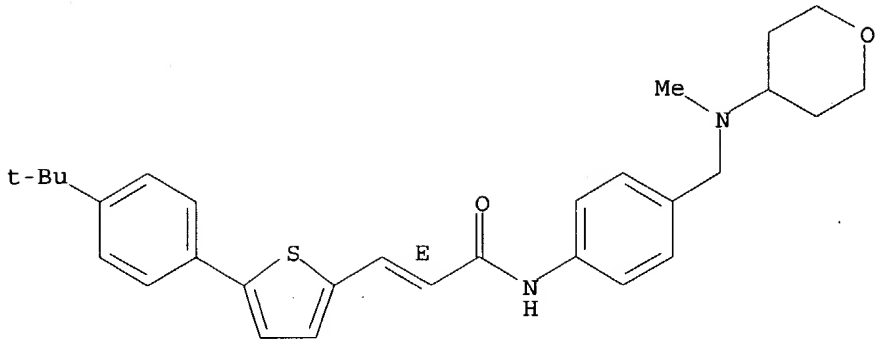
RN 229006-06-8 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



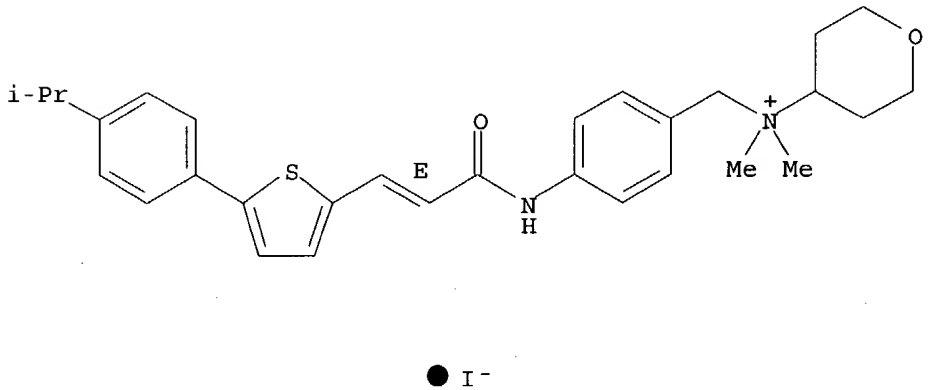
RN 229006-08-0 USPATFULL
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229006-12-6 USPATFULL
CN 2H-Pyran-4-aminium, tetrahydro-N,N-dimethyl-N-[[4-[[(2E)-3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-1-oxo-2-propenyl]amino]phenyl]methyl]-, iodide (9CI) (CA INDEX NAME)

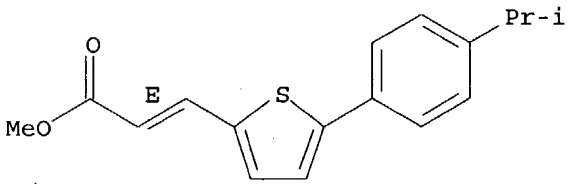
Double bond geometry as shown.



● I^-

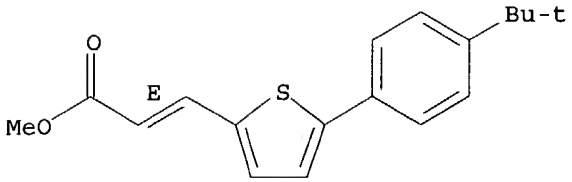
IT **229008-54-2P 229008-56-4P 229008-57-5P**
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)
RN 229008-54-2 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



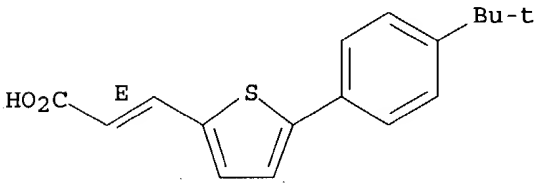
RN 229008-56-4 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229008-57-5 USPATFULL
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, (2E)-
(9CI) (CA INDEX NAME)

Double bond geometry as shown.



=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 13:59:23 ON 22 APR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 22 Apr 2004 VOL 140 ISS 17
FILE LAST UPDATED: 21 Apr 2004 (20040421/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> d all hitstr tot l48

L48 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2004:202648 HCAPLUS
ED Entered STN: 14 Mar 2004
TI Structure-Based Design of Potent Retinoid X Receptor α Agonists
AU Haffner, Curt D.; Lenhard, James M.; Miller, Aaron B.; McDougald, Darryl L.; Dwornik, Kate; Ittoop, Olivia R.; Gampe, Robert T., Jr.; Xu, H. Eric; Blanchard, Steve; Montana, Valerie G.; Consler, Tom G.; Bledsoe, Randy K.; Ayscue, Andrea; Croom, Dallas
CS GlaxoSmithKline Research and Development, Research Triangle Park, NC, 27709, USA
SO Journal of Medicinal Chemistry (2004), 47(8), 2010-2029

CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 28, 75
AB A series of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids, e.g. I, that showed potent agonist activity against RXRα were synthesized via a structure-based design approach. Among the compds. studied, I showed not only very good potency against RXRα (Ki = 6 nM) but was also found to be greater than 167-fold selective vs RARα (Ki > 1000 nM). This compound profiled out as a full agonist in a cell-based transient transfection assay (EC50 = 3 nM). The two antipodes were separated via chiral chromatog., and one was found to be 40-fold more potent than the other. Interestingly, cocrystn. of I with the RXRα protein generated a liganded structure whereby the (S)-antipode was found in the binding pocket. Given orally in db/db mice or ZDF rats, I showed a significant glucose-lowering effect and an increase in liver mass. Triglycerides decreased significantly in db/db mice but increased in the ZDF rats. A dose-dependent decrease of nonesterified free fatty acids was seen in ZDF rats but not in db/db mice. These differences indicate a species specific effect of RXR agonists on lipid metabolism
ST tetrahydrobenzofuranyl propenoic acid prepn retinoid X receptor agonist MSBAR; tetrahydrobenzothienyl propenoic acid prepn retinoid X receptor agonist MSBAR; antidiabetic agent tetrahydrobenzofuranyl tetrahydrobenzothienyl propenoic acid; antihyperglycemic activity lipid effect liver tetrahydrobenzofuranyl tetrahydrobenzothienyl propenoic acid; Complex tetrahydrobenzofuranylpropenoic acid RXR PPAR heterodimer crystal mol structure
IT INDEXING IN PROGRESS
IT Retinoic acid receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(RAR-α; prepn.of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids as antidiabetics and selective RXRα agonists verse RARα)
IT Retinoid X receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(RXRα; prepn.of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids as antidiabetics and selective RXRα agonists verse RARα)
IT Structure-activity relationship
(agonist activity against RXRα; preparation, agonist activity against RXRα, antidiabetic activity and MSBAR of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids)
IT Heterocyclic compounds
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(five-membered; preparation, agonist activity against RXRα, antidiabetic activity and MSBAR of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids)
IT Lipids
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(metabolism, lipid effect; of Complex of tetrahydrobenzofuranyl propenoic acid with RXRα:PPARγ heterodimer)
IT Crystal structure
Molecular structure
(of Complex of tetrahydrobenzofuranyl propenoic acid with RXRα:PPARγ heterodimer)
IT Antidiabetic agents
Diabetes mellitus
(preparation, agonist activity against RXRα, antidiabetic activity and MSBAR of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic

acids)

IT Carboxylic acids
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(α,β-unsatd.; preparation, agonist activity against RXRα, antidiabetic activity and MSBAR of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids)

IT 675580-33-3D, Complex with RXRα:PPARγ heterodimer
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(crystal structure; preparation, agonist activity against RXRα, antidiabetic activity and MSBAR of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids)

IT 675580-34-4P
RL: BYP (Byproduct); PREP (Preparation)
(preparation, agonist activity against RXRα, antidiabetic activity and MSBAR of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids)

IT 675579-94-9P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, agonist activity against RXRα, antidiabetic activity and MSBAR of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids)

IT 503620-55-1P 675579-95-0P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation, agonist activity against RXRα, antidiabetic activity and MSBAR of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids)

IT 503620-58-4P **675579-71-2P** 675579-96-1P 675579-97-2P
675579-98-3P 675579-99-4P 675580-02-6P 675580-03-7P 675580-04-8P
675580-08-2P 675580-17-3P 675580-30-0P 675580-32-2P 675580-37-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, agonist activity against RXRα, antidiabetic activity and MSBAR of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids)

IT 675580-35-5P 675580-36-6P
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, agonist activity against RXRα, antidiabetic activity and MSBAR of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids)

IT 498-60-2 867-13-0 1899-24-7 2295-31-0 6947-94-0 13414-95-4
16806-93-2 27452-17-1 78191-00-1 96683-92-0 119999-22-3
168082-41-5 169126-63-0 170100-73-9 201024-63-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation, agonist activity against RXRα, antidiabetic activity and MSBAR of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids)

IT 220796-18-9P 503621-20-3P 503621-21-4P 503621-28-1P 503621-29-2P
503621-30-5P 503621-31-6P 675579-69-8P **675579-70-1P**
675579-72-3P 675579-73-4P 675579-74-5P 675579-75-6P 675579-76-7P
675579-77-8P 675579-78-9P 675579-79-0P 675579-80-3P 675579-81-4P
675579-82-5P 675579-83-6P 675579-84-7P 675579-85-8P 675579-86-9P
675579-87-0P 675579-88-1P 675579-89-2P 675579-90-5P 675579-91-6P
675579-92-7P 675579-93-8P 675580-00-4P 675580-01-5P 675580-05-9P
675580-06-0P 675580-07-1P 675580-09-3P 675580-10-6P 675580-11-7P
675580-13-9P 675580-14-0P 675580-15-1P 675580-16-2P 675580-20-8P
675580-22-0P 675580-24-2P 675580-26-4P 675580-28-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, agonist activity against RXRα, antidiabetic activity and MSBAR of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids)

RE.CNT 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD

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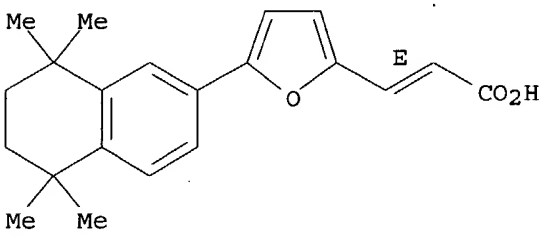
IT INDEXING IN PROGRESS

IT **675579-71-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, agonist activity against RXRα, antidiabetic activity and MSBAR of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids)

RN 675579-71-2 HCAPLUS

CN 2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-furanyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

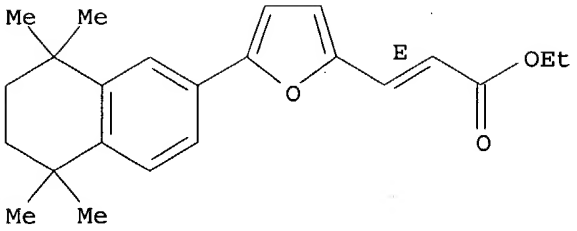


IT **675579-70-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, agonist activity against RXRα, antidiabetic activity and MSBAR of tetrahydrobenzofuranyl and tetrahydrobenzothienyl propenoic acids)

RN 675579-70-1 HCAPLUS

CN 2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-furanyl]-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L48 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:675140 HCAPLUS
DN 138:137101
ED Entered STN: 06 Sep 2002
TI Structure-Activity relationships of novel anti-Malarial agents. Part 4: N-(3-Benzoyl-4-tolylacetylaminophenyl)-3-(5-aryl-2-furyl)acrylic acid amides
AU Wiesner, Jochen; Mitsch, Andreas; Wissner, Pia; Kramer, Oliver; Jomaa, Hassan; Schlitzer, Martin
CS Biochemisches Institut der Universitatsklinik Giessen, Giessen, D-35249, Germany
SO Bioorganic & Medicinal Chemistry Letters (2002), 12(19), 2681-2683
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
OS CASREACT 138:137101
AB In a previous report, novel anti-malarial compds. based on a 2,5-diaminobenzophenone scaffold were described. Here, acryloyl derivs. carrying a biaryl structure consisting of a terminal aryl residue and a central 2-furyl ring were investigated. Several compds. were obtained in the series of para-substituted phenylfurylacryloyl derivs. that displayed improved anti-malarial activity in comparison to earlier described derivs. From the structure-activity relationships it can be deduced that there has to be a lipophilic moiety in the para-position of the terminal Ph residue. Furthermore, there are indications that, alternatively, activity may benefit from the presence of a polar moiety with hydrogen bond acceptor properties.
ST acryloyl deriv biaryl furyl prepn; antimalarial acryloyl deriv prepn; benzoyltolylacetylaminophenyl aryl furyl acrylic acid amide prepn
IT Structure-activity relationship
(antimalarial; preparation of biaryl acryloyl derivs. from 5-bromofurfural and evaluation of antimalarial activity)
IT Antimalarials
(preparation of biaryl acryloyl derivs. from 5-bromofurfural and evaluation of antimalarial activity)
IT 493037-15-3P 493037-16-4P **493037-17-5P** 493037-18-6P
493037-19-7P 493037-20-0P **493037-21-1P** 493037-22-2P
493037-23-3P 493037-24-4P 493037-25-5P 493037-26-6P 493037-27-7P
493037-28-8P 493037-29-9P 493037-30-2P 493037-31-3P 493037-32-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of biaryl acryloyl derivs. from 5-bromofurfural and evaluation of antimalarial activity)
IT 98-80-6 1679-18-1 1765-93-1 1899-24-7 2156-04-9 5467-74-3
5570-19-4 5720-05-8 5720-07-0 13331-27-6 13922-41-3 22237-13-4
24067-17-2 32316-92-0 63139-21-9 98546-51-1 123324-71-0
139301-27-2 186497-67-6
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of biaryl acryloyl derivs. from 5-bromofurfural and evaluation of antimalarial activity)

IT 141-82-2, Malonic acid, reactions 265648-28-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant)

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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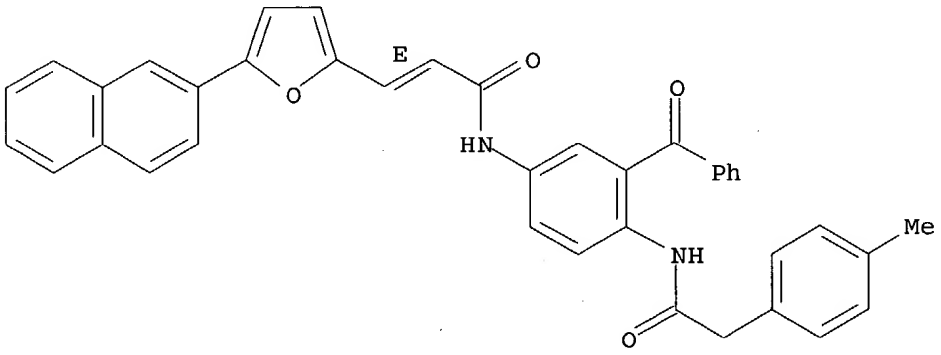
(10) Wiesner, J; Bioorg Med Chem 2001, V9, P785 HCAPLUS
(11) Wiesner, J; Bioorg Med Chem Lett 2001, V11, P423 HCAPLUS

IT **493037-17-5P 493037-21-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of biaryl acryloyl derivs. from 5-bromofurfural and evaluation of antimalarial activity)

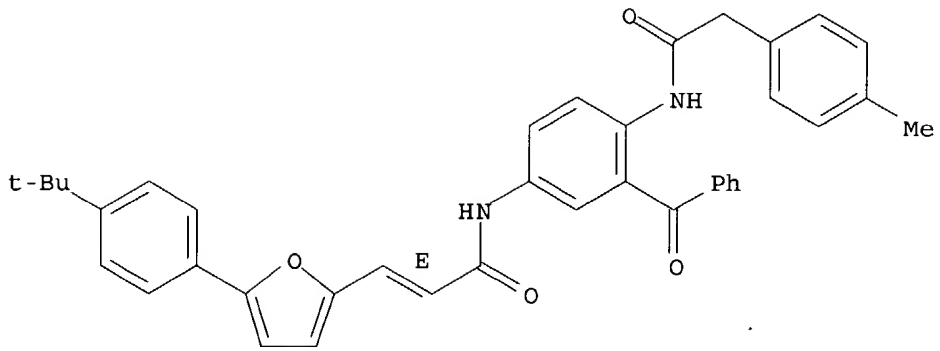
RN 493037-17-5 HCAPLUS
CN Benzeneacetamide, N-[2-benzoyl-4-[[(2E)-3-[5-(2-naphthalenyl)-2-furanyl]-1-oxo-2-propenyl]amino]phenyl]-4-methyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 493037-21-1 HCAPLUS
CN Benzeneacetamide, N-[2-benzoyl-4-[[(2E)-3-[5-[4-(1,1-dimethylethyl)phenyl]-2-furanyl]-1-oxo-2-propenyl]amino]phenyl]-4-methyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L48 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:338368 HCAPLUS
DN 133:135199
ED Entered STN: 23 May 2000
TI Facile Synthesis of Oxa- and Azacyclic Dienes via Cycloalkenation of Alkynyltungsten Compounds. Stereoselective Construction of Tricyclic Furan and Pyran Derivatives via Intramolecular Diels-Alder Reaction
AU Li, Wen-Tai; Pan, Min-Hui; Wu, Yi-Ru; Wang, Sue-Lein; Liao, Fen-Lin; Liu, Rai-Shung
CS Department of Chemistry, National Tsing-Hua University, Hsinchu, Taiwan
SO Journal of Organic Chemistry (2000), 65(12), 3761-3766
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 29
OS CASREACT 133:135199
AB A convenient and short synthesis of functionalized oxacyclic and azacyclic dienes is developed on the basis of organotungsten chemical Alkynyltungsten compds. bearing a tethered alc. and amine are treated with aldehydes and BF3.Et2O in cold di-Et ether to give tungsten-heterocyclic carbenium salts, further leading to tungsten-heterocyclic dienes via deprotonation with Et3N. Hydrodemetalation of these tungsten-heterocyclic dienes is performed by the action of anhydrous Me3NO in MeCN. This method is applicable to the synthesis of a number of oxa- and azacyclic dienes, including those tethered with an electron-deficient olefin. The oxacyclic 1,3,8-nonatrienes and 1,3,9-decatrienes undergo intramol. Diels-Alder reactions upon heating in toluene, yielding tricyclic tetrahydropyran and -furan derivs. with excellent diastereoselectivities.
ST pyran tetrahydro tricyclic prepn; furan tetrahydro tricyclic prepn; pyrrole alkenyl prepn; tungsten furyl pyranyl pyrrolyl prepn demetalation; alkynyltungsten reaction aldehyde
IT Diels-Alder reaction
(intramol.; stereoselective preparation of tricyclic furans and pyran via cycloalkenation of alkynyltungsten compds. and intramol. Diels-Alder reaction)
IT Cyclocondensation reaction
(stereoselective preparation of tricyclic furans and pyran via cycloalkenation of alkynyltungsten compds. and intramol. Diels-Alder reaction)
IT Heterocyclic compounds
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of tricyclic furans and pyran via cycloalkenation of alkynyltungsten compds. and intramol. Diels-Alder reaction)

IT 285565-50-6P 285565-61-9P 285565-62-0P 285565-63-1P 285565-64-2P
285565-65-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of tricyclic furans and pyran via cycloalkenation of alkynyltungsten compds. and intramol. Diels-Alder reaction)

IT 108-31-6, Maleic anhydride, reactions 541-59-3, Maleimide 624-48-6, Dimethyl maleate 941-69-5 1423-60-5, 3-Butyn-2-one 12128-24-4 190448-89-6 205755-53-9 285565-39-1 285565-55-1 285565-67-5 285565-68-6 286426-97-9 286426-98-0 286426-99-1 286427-00-7 286427-01-8 286427-03-0 286427-11-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective preparation of tricyclic furans and pyran via cycloalkenation of alkynyltungsten compds. and intramol. Diels-Alder reaction)

IT 285565-43-7P 285565-56-2P 285565-57-3P 285565-58-4P 285565-59-5P 285565-60-8P 286426-93-5P 286426-95-7P 286426-96-8P 286427-05-2P 286427-08-5P 286427-10-9P 286427-13-2P 286427-14-3P 286427-16-5P 286427-17-6P 286427-19-8P 286427-20-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation of tricyclic furans and pyran via cycloalkenation of alkynyltungsten compds. and intramol. Diels-Alder reaction)

IT 285565-40-4P 285565-41-5P 285565-42-6P 285565-44-8P 285565-45-9P 285565-46-0P 285565-47-1P 285565-48-2P 285565-49-3P 285565-51-7P 285565-52-8P 285565-53-9P 285565-54-0P **285565-66-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of tricyclic furans and pyran via cycloalkenation of alkynyltungsten compds. and intramol. Diels-Alder reaction)

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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(3) Boeckman, R; J Am Chem Soc 1988, V110, P8250 HCAPLUS
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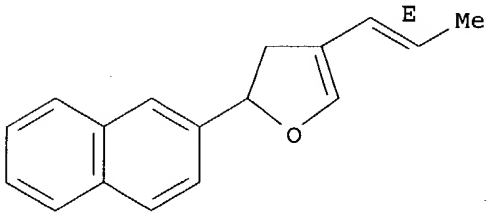
(23) Trost, B; J Am Chem Soc 1984, V106, P7641 HCAPLUS
(24) Wu, T; Tetrahedron Lett 1985, V26, P2293 HCAPLUS

IT **285565-66-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of tricyclic furans and pyran via cycloalkenation of alkynyltungsten compds. and intramol. Diels-Alder reaction)

RN 285565-66-4 HCAPLUS

CN Furan, 2,3-dihydro-2-(2-naphthalenyl)-4-(1E)-1-propenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L48 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:421672 HCAPLUS
DN 131:73571
ED Entered STN: 08 Jul 1999
TI Preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compounds as MCP-1 receptor antagonists.
IN Shiraishi, Mitsuru; Kitayoshi, Takahito; Aramaki, Yoshio; Honda, Susumu; Oda, Tsuneo
PA Takeda Chemical Industries, Ltd., Japan
SO PCT Int. Appl., 513 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D295-12
ICS A61K031-16; A61K031-33; A61K031-66; C07C233-62; C07D213-20; C07D213-61; C07D213-84; C07D213-85; C07F009-44; C07F009-54; C07F009-6584; C07F009-6568; C07F009-655; C07F009-53; C07D313-08; C07D407-12
CC 27-21 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 25, 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9932468	A1	19990701	WO 1998-JP5707	19981217
	W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	BR 9813686	A	20001010	BR 1998-13686	19981212
	CA 2311428	AA	19990701	CA 1998-2311428	19981217
	AU 9916830	A1	19990712	AU 1999-16830	19981217
	AU 742077	B2	20011213		
	ZA 9811576	A	20000619	ZA 1998-11576	19981217
	EP 1040103	A1	20001004	EP 1998-961383	19981217
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	US 6166006	A	20001226	US 1998-213379	19981217
	JP 11263764	A2	19990928	JP 1998-360780	19981218
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	US 6413947	B1	20020702	US 2000-661194	20000913
PRAI	JP 1997-351481	A	19971219		
	US 1998-213379	A3	19981217		
	WO 1998-JP5707	W	19981217		

OS MARPAT 131:73571
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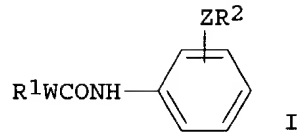

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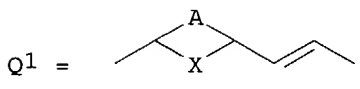

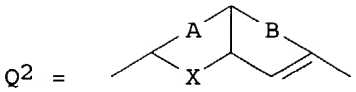

AB Title compds. I [R1 = (substituted) 5-6 membered ring; W = Q1, Q2; A = atoms to form a (substituted) 5-6 membered aromatic ring; X = S, O, (substituted) C, N; B = atoms to form a (substituted) 5-7 membered ring; Z = bond, divalent group; R2 = (substituted) amino, ammonio, heterocyclyl, S-bonded group, P(O)kR5R6; k = 0, 1; R5, R6 = (substituted) hydrocarbyl, amino; PR5R6 = cyclic group], were prepared Thus, 7-(4-methylphenyl)-2,3-dihydro-1-benzoxepine-4-carboxylic acid in CH2Cl2 was treated with (COCl)2 and DMF to give a residue which was stirred with 4-[N-methyl-N-(tetrahydropyran-4-yl)aminomethyl]aniline and Et3N in THF to give N-[4-[N-methyl-N-(tetrahydropyran-4-yl)aminomethyl]phenyl]-7-(4-methylphenyl)-2,3-dihydro-1-benzoxepine-4-carboxamide (II). II at 1 μM inhibited MCP-1 induced chemotaxis in CHO cells by 89%. A II capsule composition is given.

ST benzoxepinecarboxamide prepn monocyte chemoattractant protein receptor antagonist; benzocycloheptenecarboxamide prepn monocyte chemoattractant protein receptor antagonist; naphthalenecarboxamide prepn monocyte chemoattractant protein receptor antagonist; myocarditis treatment benzoxepinecarboxamide benzocycloheptenecarboxamide naphthalenecarboxamide; cardiac infarction treatment benzoxepinecarboxamide benzocycloheptenecarboxamide naphthalenecarboxamide

IT Monocyte chemoattractant protein-1
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(antagonists; preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Heart, disease
(infarction, treatment; preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Chemokine receptors
Chemokine receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(monocyte chemoattractant protein-1; preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Heart, disease
(myocarditis, treatment; preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 229003-88-7P 229004-17-5P 229004-21-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides,

naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 229003-36-5P 229003-37-6P 229003-38-7P 229003-39-8P 229003-40-1P
229003-41-2P 229003-42-3P 229003-43-4P 229003-44-5P 229003-45-6P
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229005-39-4P 229005-40-7P 229005-41-8P 229005-42-9P 229005-43-0P
229005-44-1P 229005-45-2P 229005-46-3P 229005-47-4P 229005-48-5P
229005-49-6P 229005-50-9P 229005-51-0P 229005-52-1P 229005-53-2P
229005-54-3P 229005-55-4P 229005-56-5P 229005-57-6P 229005-58-7P
229005-59-8P 229005-60-1P 229005-61-2P 229005-62-3P 229005-63-4P
229005-64-5P 229005-65-6P 229005-66-7P 229005-67-8P 229005-68-9P
229005-69-0P 229005-70-3P 229005-71-4P 229005-72-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 229005-73-6P 229005-74-7P 229005-75-8P 229005-76-9P 229005-77-0P
229005-78-1P 229005-79-2P 229005-80-5P 229005-81-6P 229005-82-7P
229005-83-8P 229005-84-9P 229005-85-0P 229005-86-1P 229005-87-2P
229005-88-3P 229005-89-4P 229005-90-7P 229005-91-8P 229005-92-9P
229005-93-0P 229005-94-1P 229005-95-2P 229005-96-3P 229005-97-4P
229005-98-5P 229005-99-6P 229006-00-2P **229006-01-3P**
229006-02-4P 229006-03-5P 229006-04-6P 229006-05-7P
229006-06-8P 229006-07-9P **229006-08-0P** 229006-09-1P

229006-10-4P 229006-11-5P **229006-12-6P** 229006-13-7P
229006-14-8P 229006-15-9P 229006-16-0P 229006-17-1P 229006-18-2P
229006-19-3P 229006-20-6P 229006-21-7P 229006-22-8P 229006-23-9P
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229006-39-7P 229006-40-0P 229006-41-1P 229006-42-2P 229006-43-3P
229006-44-4P 229006-45-5P 229006-46-6P 229006-47-7P 229006-48-8P
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229009-44-3P 229009-45-4P 229009-46-5P 229009-47-6P 229153-64-4P
229153-65-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 75-64-9, tert-Butylamine, reactions 76-05-1, reactions 78-67-1 96-22-0, 3-Pentanone 96-97-9 98-53-3, 4-tert-Butylcyclohexanone 99-98-9, 4-Dimethylaminoaniline 100-11-8, 4-Nitrobenzylbromide 100-14-1, 4-Nitrobenzylchloride 100-48-1, 4-Cyanopyridine 100-54-9, 3-Cyanopyridine 100-60-7, N-Cyclohexyl-N-methylamine 100-61-8, N-Methylaniline, reactions 100-76-5, Quinuclidine 102-69-2, Tripropylamine 103-67-3, N-Methylbenzylamine 103-76-4, 1-(2-Hydroxyethyl)piperazine 106-41-2, 4-Bromophenol 106-53-6, 4-Bromothiophenol 107-08-4 107-15-3, 1,2-Ethanediamine, reactions 108-94-1, Cyclohexanone, reactions 108-99-6, 3-Picoline 109-01-3, 1-Methylpiperazine 109-04-6, 2-Bromopyridine 109-06-8, 2-Picoline 110-52-1, 1,4-Dibromobutane 110-68-9, N-Methyl-N-butylamine 110-87-2 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 111-24-0, 1,5-Dibromopentane 111-33-1 111-42-2, reactions 111-49-9 111-96-6, Bis(2-methoxyethyl)ether 120-92-3, Cyclopentanone 121-44-8, reactions 122-00-9 123-75-1, Pyrrolidine, reactions 123-90-0, Thiomorpholine 288-47-1, Thiazole 358-23-6, Trifluoromethanesulfonic acid anhydride 407-14-7, 4-Trifluoromethoxybromobenzene 462-08-8, 3-Aminopyridine 497-38-1, Norcamphor 502-42-1, Cycloheptanone 534-03-2, 2-Amino-1,3-propanediol 536-78-7, 3-Ethylpyridine 539-88-8, Ethyl levulinate 555-16-8, 4-Nitrobenzaldehyde, reactions 585-70-6, 5-Bromo-2-furancarboxylic acid 588-96-5, 4-Bromophenetole 591-22-0, 3,5-Lutidine 591-49-1, 1-Methylcyclohexene 616-44-4 617-05-0, Ethyl vanillate 617-27-6 619-23-8, 3-Nitrobenzyl chloride 619-73-8, 4-Nitrobenzylalcohol 620-87-1, 2-(4-Nitrobenzyl)pyridine 625-43-4, N-Methylisobutylamine 626-60-8, 3-Chloropyridine 626-67-5, 1-Methylpiperidine 765-58-2, 5-Bromo-2-methylthiophene 766-09-6, 1-Ethylpiperidine 766-97-2, 4-Methylphenylacetylene 771-99-3, 4-Phenylpiperidine 841-77-0, 1-Benzhydrylpiperazine 930-69-8, Sodium phenylsulfide 998-40-3, Tributylphosphine 1003-09-4, 2-Bromothiophene 1072-72-6, 4H-Tetrahydrothiopyran-4-one 1080-32-6, Diethyl benzylphosphonate 1121-92-2 1205-62-5, 4-Nitrobenzylphosphonic acid 1450-75-5 1484-84-0, 2-(2-Hydroxyethyl)piperidine 1585-07-5, 4-Ethylbromobenzene 1663-39-4 1679-18-1, 4-Chlorophenylboronic acid 1692-15-5 1722-12-9, 2-Chloropyrimidine 1761-61-1, 5-Bromosalicylaldehyde 1765-93-1, 4-Fluorophenylboronic acid 2320-30-1, 3,5-Dimethylcyclohexanone 2338-18-3 2605-67-6 2635-13-4 2969-81-5, Ethyl-4-bromobutyrate 3132-99-8, 3-Bromobenzaldehyde 3218-02-8, Amino-methylcyclohexane 3287-99-8, Benzylamine hydrochloride 3433-37-2, 2-Piperidinemethanol 3490-06-0 3492-64-6 4068-76-2, Methyl-5-bromosalicylate 4606-65-9, 3-(Hydroxymethyl)piperidine 4701-17-1, 5-Bromo-2-thiophenecarboxaldehyde 4746-97-8, 1,4-Cyclohexanedione monoethyleneketal 5105-78-2 5205-39-0 5332-73-0, 3-Methoxypropylamine 5339-26-4, 4-(2-Bromoethyl)nitrobenzene 5382-16-1, 4-Hydroxypiperidine 5459-93-8, N-Ethylcyclohexylamine 5466-06-8, Ethyl 3-mercaptopropionate 5720-05-8, 4-Methylphenylboronic

acid 5794-88-7, 5-Bromoanthranilic acid 6165-69-1 6291-85-6, 3-Ethoxypropylamine 6388-74-5, p-Nitrostyreneoxide 6602-32-0, 2-Bromo-3-hydroxypyridine 6638-79-5, N,O-Dimethylhydroxylamine hydrochloride 6836-19-7, 7-Methoxy-1-tetralone 6850-65-3, 4-Aminocyclohexanol 6859-99-0, 3-Hydroxypiperidine 10544-63-5, Ethyl crotonate 13331-23-2, 2-Furylboronic acid 13331-27-6, 3-Nitrophenylboronic acid 13515-93-0, Sarcosine methyl ester hydrochloride 13623-25-1, 6-Methoxy-1-indanone 13952-84-6, 1-Methylpropylamine 15300-97-7 16419-60-6 17857-14-6, (3-Carboxypropyl)triphenylphosphonium bromide 18471-73-3, 2-(4-Aminophenyl)pyridine 18600-42-5, p-Nitrobenzylamine hydrochloride 18664-32-9, 1,3-Dimethoxyacetone 18791-75-8, 4-Bromo-2-thiophenecarboxaldehyde 20074-79-7, Diethyl 4-aminobenzylphosphonate 20826-04-4, 5-Bromonicotinic acid 20980-22-7, 1-(2-Pyrimidyl)piperazine 23462-75-1, Tetrahydropyran-3-one 24252-37-7, Ethyl 1-methylpiperidine-4-carboxylate 25808-30-4 28611-39-4 29943-42-8, 4H-Tetrahydropyran-4-one 31252-42-3, 4-Benzylpiperidine 32231-06-4, 1-(3,4-Methylenedioxybenzyl)-piperazine 35386-24-4, 1-(2-Methoxyphenyl)piperazine 38212-30-5, 1-(4-Methoxyphenyl)piperazine 50541-93-0, 4-Amino-1-benzylpiperidine 50729-68-5 52146-35-7, 1-(3,4,5-Trimethoxybenzyl)piperazine 60548-09-6, 1-(2-Furoyl)piperazine hydrochloride 61081-32-1 73579-08-5, 1-Methyl-4-methylaminopiperidine 79099-07-3 80670-21-9 82261-42-5, 3-(4-Aminophenyl)pyridine 85199-06-0 87779-78-0 89878-14-8, Diethyl-(3-pyridyl)-borane 93777-26-5, 5-Bromo-2-fluorobenzaldehyde 96251-92-2 98546-51-1, 4-Methylthiophenylboronic acid 128796-39-4, 4-Trifluoromethylphenylboronic acid 162210-31-3 162271-10-5 175394-06-6 186498-02-2 229009-38-5 229009-39-6 229009-40-9 229009-41-0 229009-42-1 229009-43-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 623-04-1P, 4-Aminobenzyl alcohol 955-44-2P 2089-33-0P 2439-56-7P 4519-78-2P, Benzyldiethylphosphine oxide 5339-15-1P 6149-46-8P 6406-74-2P 6425-46-3P 6763-91-3P 6881-57-8P, Benzylphosphonic acid 14473-91-7P 15084-55-6P 15115-76-1P 15184-96-0P 16341-77-8P 17302-46-4P 18483-99-3P 18484-05-4P 20173-88-0P 20712-12-3P 22009-38-7P, 7-Hydroxy-1-tetralone 22237-13-4P, 4-Ethoxyphenylboronic acid 24100-18-3P 29124-57-0P 29608-05-7P 34035-05-7P 34160-40-2P 38035-10-8P 40594-34-1P 41526-73-2P, 7-Phenyl-1-tetralone 42870-65-5P 50534-23-1P 50534-24-2P 51013-67-3P 53678-61-8P 54306-15-9P 55008-98-5P 55009-03-5P 55580-07-9P 55580-08-0P 56851-32-2P 58498-12-7P 59507-44-7P 59507-46-9P 59719-62-9P 62157-62-4P 62803-47-8P, 6-Hydroxy-1-indanone 62806-32-0P 63139-21-9P, 4-Ethylphenylboronic acid 73676-23-0P 79432-87-4P 79909-21-0P 83619-74-3P 91150-58-2P 91953-92-3P 92033-77-7P 93138-55-7P 94839-07-3P 95323-86-7P 98008-66-3P 123324-71-0P, 4-tert-Butylphenylboronic acid 131230-76-7P 133851-67-9P 135605-97-9P 138007-25-7P 139301-27-2P, 4-Trifluoromethoxyphenylboronic acid 142335-64-6P 143632-57-9P 144464-65-3P 145654-38-2P 147539-41-1P 160127-63-9P 162607-15-0P 162607-20-7P 168897-21-0P 175393-25-6P 175394-17-9P 175840-02-5P 179055-22-2P 183608-47-1P 185111-27-7P 229006-54-6P 229006-55-7P 229006-56-8P 229006-57-9P 229006-58-0P 229006-59-1P 229006-60-4P 229006-61-5P 229006-62-6P 229006-63-7P 229006-64-8P 229006-65-9P 229006-66-0P 229006-67-1P 229006-68-2P 229006-69-3P 229006-70-6P 229006-71-7P 229006-72-8P 229006-73-9P 229006-74-0P 229006-75-1P 229006-76-2P 229006-77-3P 229006-78-4P 229006-79-5P 229006-80-8P 229006-81-9P 229006-82-0P 229006-83-1P 229006-84-2P 229006-85-3P 229006-86-4P 229006-87-5P 229006-88-6P 229006-89-7P 229006-90-0P 229006-91-1P 229006-92-2P 229006-93-3P 229006-94-4P 229006-95-5P 229006-96-6P 229006-97-7P 229006-98-8P 229006-99-9P 229007-00-5P

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229007-81-2P 229007-82-3P 229007-83-4P 229007-84-5P 229007-85-6P
229007-86-7P 229007-87-8P 229007-88-9P 229007-89-0P 229007-90-3P
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229007-96-9P 229007-97-0P 229007-98-1P 229007-99-2P 229008-00-8P
229008-01-9P 229008-02-0P 229008-03-1P 229008-04-2P 229008-05-3P
229008-06-4P 229008-07-5P 229008-09-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 229008-11-1P 229008-14-4P 229008-16-6P 229008-18-8P 229008-20-2P
229008-22-4P 229008-24-6P 229008-26-8P 229008-27-9P 229008-28-0P
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229008-34-8P 229008-35-9P 229008-36-0P 229008-37-1P 229008-38-2P
229008-39-3P 229008-40-6P 229008-41-7P 229008-42-8P 229008-43-9P
229008-44-0P 229008-45-1P 229008-46-2P 229008-47-3P 229008-48-4P
229008-49-5P 229008-50-8P 229008-51-9P 229008-52-0P 229008-53-1P
229008-54-2P 229008-55-3P **229008-56-4P**
229008-57-5P 229008-58-6P 229008-59-7P 229008-60-0P
229008-61-1P 229008-62-2P 229008-63-3P 229008-64-4P 229008-65-5P
229008-66-6P 229008-67-7P 229008-68-8P 229008-69-9P 229008-70-2P
229008-71-3P 229008-72-4P 229008-73-5P 229008-74-6P 229008-75-7P
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229008-96-2P 229008-97-3P 229008-98-4P 229008-99-5P 229009-00-1P
229009-01-2P 229009-02-3P 229009-03-4P 229009-04-5P 229009-05-6P
229009-06-7P 229009-07-8P 229009-08-9P 229009-09-0P 229009-10-3P
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229009-16-9P 229009-17-0P 229009-18-1P 229009-19-2P 229009-20-5P
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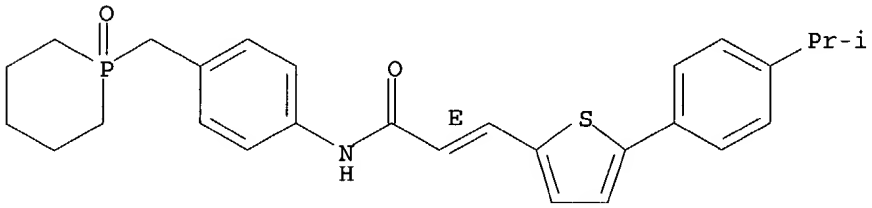
229009-26-1P 229009-27-2P 229009-28-3P 229009-29-4P 229009-30-7P
229009-31-8P 229009-32-9P 229009-33-0P 229009-34-1P 229009-35-2P
229009-36-3P 229009-37-4P 229153-66-6P 229153-67-7P 229153-68-8P
229153-69-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Teijin Ltd; JP 07025756 A 1995 HCAPLUS
(2) Teijin Ltd; JP 07025757 A 1995 HCAPLUS
IT **229006-01-3P 229006-02-4P 229006-06-8P**

229006-08-0P 229006-12-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

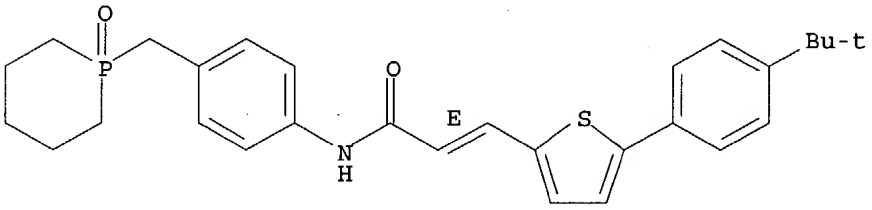
RN 229006-01-3 HCAPLUS
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



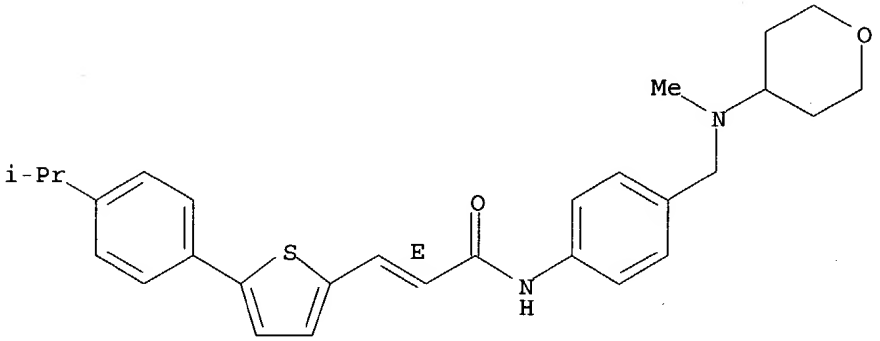
RN 229006-02-4 HCAPLUS
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229006-06-8 HCAPLUS
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

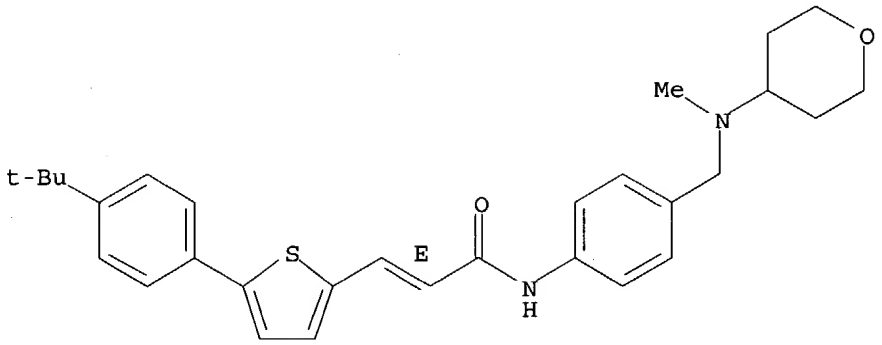
Double bond geometry as shown.



RN 229006-08-0 HCAPLUS
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA

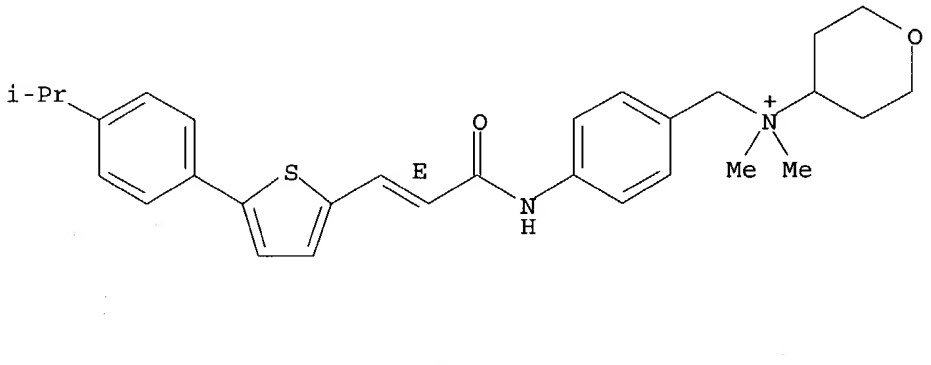
INDEX NAME)

Double bond geometry as shown.



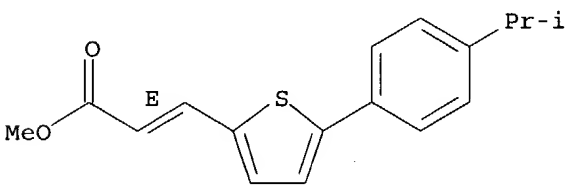
RN 229006-12-6 HCAPLUS
CN 2H-Pyran-4-aminium, tetrahydro-N,N-dimethyl-N-[[4-[[(2E)-3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-1-oxo-2-propenyl]amino]phenyl]methyl]-, iodide (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT **229008-54-2P 229008-56-4P 229008-57-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)
RN 229008-54-2 HCAPLUS
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

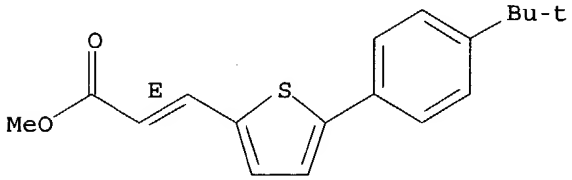
Double bond geometry as shown.



RN 229008-56-4 HCAPLUS

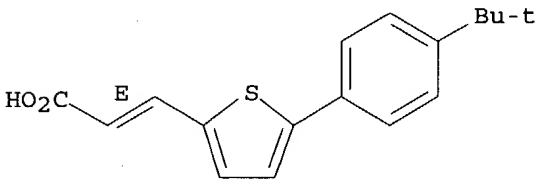
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229008-57-5 HCAPLUS
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L48 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:421562 HCAPLUS
DN 131:87834
ED Entered STN: 08 Jul 1999
TI Preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compounds as CCR5 antagonists.
IN Nishimura, Osamu; Baba, Masanori; Sawada, Hidekazu; Kanzaki, Naoyuki; Kuroshima, Ken-ichi; Shiraishi, Mitsuru; Aramaki, Yoshio
PA Takeda Chemical Industries, Ltd., Japan
SO PCT Int. Appl., 516 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K031-00
CC 27-21 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 25, 63
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9932100	A2	19990701	WO 1998-JP5708	19981217
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	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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	AU 9916831	A1	19990712	AU 1999-16831	19981217
	AU 748064	B2	20020530		
	ZA 9811574	A	20000619	ZA 1998-11574	19981217
	EP 1039899	A2	20001004	EP 1998-961384	19981217

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI

	BR 9813691	A	20001010	BR 1998-13691	19981217
	JP 2000128782	A2	20000509	JP 1998-360820	19981218
	US 6096780	A	20000801	US 1999-377040	19990819
	US 6376536	B1	20020423	US 2000-580270	20000526
	NO 2000003179	A	20000619	NO 2000-3179	20000619
	US 6268354	B1	20010731	US 2000-661320	20000913
PRAI	JP 1997-351480	A	19971219		
	JP 1998-218875	A	19980803		
	JP 1998-234388	A	19980820		
	US 1998-104845P	P	19981016		
	US 1998-104847P	P	19981116		
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	WO 1998-JP5708	W	19981217		
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OS MARPAT 131:87834

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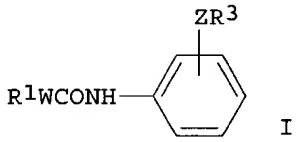

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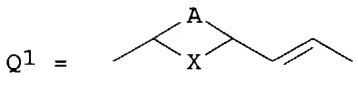

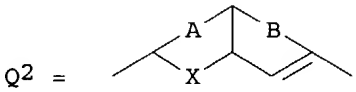

AB A pharmaceutical composition for antagonizing CCR5 comprises I [R1 = (substituted) 5-6 membered ring; W = Q1, Q2; A = atoms to form a (substituted) 5-6 membered aromatic ring; X = S, O, (substituted) C, N; B = atoms to form a (substituted) 5-7 membered ring; Z = bond, divalent group; R2 = (substituted) amino, ammonio, heterocyclyl, S-bonded group, P(O)kR5R6; k = 0, 1; R5, R6 = (substituted) hydrocarbyl, amino; PR5R6 = cyclic group]. Thus, 7-(4-methylphenyl)-2,3-dihydro-1-benzoxepine-4-carboxylic acid in CH2Cl2 was treated with (COCl)2 and DMF to give a residue which was stirred with 4-[N-methyl-N-(tetrahydropyran-4-yl)aminomethyl]aniline and Et3N in THF to give N-[4-[N-methyl-N-(tetrahydropyran-4-yl)aminomethyl]phenyl]-7-(4-methylphenyl)-2,3-dihydro-1-benzoxepine-4-carboxamide (II). A II capsule composition is given.

ST benzoxepinecarboxamide prepn chemokine coreceptor antagonist; benzocycloheptenecarboxamide prepn chemokine coreceptor antagonist; naphthalenecarboxamide prepn chemokine coreceptor antagonist; AIDS treatment benzoxepinecarboxamide benzocycloheptenecarboxamide naphthalenecarboxamide

IT Monocyte chemoattractant protein-1
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(antagonists; preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Chemokine receptors
Chemokine receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(monocyte chemoattractant protein-1; preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Anti-AIDS agents
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Chemokine receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(β chemokine receptor CCR5; preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT Chemokines
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(β, receptor CCR5; preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 229003-88-7P 229004-17-5P 229004-21-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 229003-36-5P 229003-37-6P 229003-38-7P 229003-39-8P 229003-40-1P
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229005-69-0P 229005-70-3P 229005-71-4P 229005-72-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 229005-73-6P 229005-74-7P 229005-75-8P 229005-76-9P 229005-77-0P
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 75-64-9, tert-Butylamine, reactions 76-05-1, reactions 78-67-1
96-22-0, 3-Pentanone 96-97-9 98-53-3, 4-tert-Butylcyclohexanone
99-98-9, 4-Dimethylaminoaniline 100-11-8, 4-Nitrobenzylbromide
100-14-1, 4-Nitrobenzylchloride 100-48-1, 4-Cyanopyridine 100-54-9,
3-Cyanopyridine 100-60-7, N-Cyclohexyl-N-methylamine 100-61-8,
N-Methylaniline, reactions 100-76-5, Quinuclidine 102-69-2,
Tripropylamine 103-67-3, N-Methylbenzylamine 103-76-4,
1-(2-Hydroxyethyl)piperazine 106-41-2, 4-Bromophenol 106-53-6,
4-Bromothiophenol 107-08-4 107-15-3, 1,2-Ethanediamine, reactions
108-94-1, Cyclohexanone, reactions 108-99-6, 3-Picoline 109-01-3,
1-Methylpiperazine 109-04-6, 2-Bromopyridine 109-06-8, 2-Picoline
110-52-1, 1,4-Dibromobutane 110-68-9, N-Methyl-N-butylamine 110-87-2
110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions
111-24-0, 1,5-Dibromopentane 111-33-1 111-42-2, reactions 111-49-9
111-96-6, Bis(2-methoxyethyl)ether 120-92-3, Cyclopentanone 121-44-8,
reactions 122-00-9 123-75-1, Pyrrolidine, reactions 123-90-0,
Thiomorpholine 288-47-1, Thiazole 358-23-6, Trifluoromethanesulfonic
acid anhydride 407-14-7, 4-Trifluoromethoxybromobenzene 462-08-8,
3-Aminopyridine 497-38-1, Norcamphor 502-42-1, Cycloheptanone
534-03-2, 2-Amino-1,3-propanediol 536-78-7, 3-Ethylpyridine 539-88-8,
Ethyl levulinate 555-16-8, 4-Nitrobenzaldehyde, reactions 585-70-6,
5-Bromo-2-furancarboxylic acid 588-96-5, 4-Bromophenetole 591-22-0,
3,5-Lutidine 591-49-1, 1-Methylcyclohexene 616-44-4 617-05-0, Ethyl
vanillate 617-27-6 619-23-8, 3-Nitrobenzyl chloride 619-73-8,

4-Nitrobenzylalcohol 620-87-1, 2-(4-Nitrobenzyl)pyridine 625-43-4, N-Methylisobutylamine 626-60-8, 3-Chloropyridine 626-67-5, 1-Methylpiperidine 765-58-2, 5-Bromo-2-methylthiophene 766-09-6, 1-Ethylpiperidine 766-97-2, 4-Methylphenylacetylene 771-99-3, 4-Phenylpiperidine 841-77-0, 1-Benzhydrylpiperazine 930-69-8, Sodium phenylsulfide 998-40-3, Tributylphosphine 1003-09-4, 2-Bromothiophene 1072-72-6, 4H-Tetrahydrothiopyran-4-one 1080-32-6, Diethyl benzylphosphonate 1121-92-2 1205-62-5, 4-Nitrobenzylphosphonic acid 1450-75-5 1484-84-0, 2-(2-Hydroxyethyl)piperidine 1585-07-5, 4-Ethylbromobenzene 1663-39-4 1679-18-1, 4-Chlorophenylboronic acid 1692-15-5 1722-12-9, 2-Chloropyrimidine 1761-61-1, 5-Bromosalicylaldehyde 1765-93-1, 4-Fluorophenylboronic acid 2320-30-1, 3,5-Dimethylcyclohexanone 2338-18-3 2605-67-6 2635-13-4 2969-81-5, Ethyl-4-bromobutyrate 3132-99-8, 3-Bromobenzaldehyde 3218-02-8, Amino-methylcyclohexane 3287-99-8, Benzylamine hydrochloride 3433-37-2, 2-Piperidinemethanol 3490-06-0 3492-64-6 4068-76-2, Methyl-5-bromosalicylate 4606-65-9, 3-(Hydroxymethyl)piperidine 4701-17-1, 5-Bromo-2-thiophenecarboxaldehyde 4746-97-8, 1,4-Cyclohexanedione monoethyleneketal 5105-78-2 5205-39-0 5332-73-0, 3-Methoxypropylamine 5339-26-4, 4-(2-Bromoethyl)nitrobenzene 5382-16-1, 4-Hydroxypiperidine 5459-93-8, N-Ethylcyclohexylamine 5466-06-8, Ethyl 3-mercaptopropionate 5720-05-8, 4-Methylphenylboronic acid 5794-88-7, 5-Bromoanthranilic acid 6165-69-1 6291-85-6, 3-Ethoxypropylamine 6388-74-5, p-Nitrostyreneoxide 6602-32-0, 2-Bromo-3-hydroxypyridine 6638-79-5, N,O-Dimethylhydroxylamine hydrochloride 6836-19-7, 7-Methoxy-1-tetralone 6850-65-3, 4-Aminocyclohexanol 6859-99-0, 3-Hydroxypiperidine 10544-63-5, Ethyl crotonate 13331-23-2, 2-Furylboronic acid 13331-27-6, 3-Nitrophenylboronic acid 13515-93-0, Sarcosine methyl ester hydrochloride 13623-25-1, 6-Methoxy-1-indanone 13952-84-6, 1-Methylpropylamine 15300-97-7 16419-60-6 17857-14-6, (3-Carboxypropyl)triphenylphosphonium bromide 18471-73-3, 2-(4-Aminophenyl)pyridine 18600-42-5, p-Nitrobenzylamine hydrochloride 18664-32-9, 1,3-Dimethoxyacetone 18791-75-8, 4-Bromo-2-thiophenecarboxaldehyde 20074-79-7, Diethyl 4-aminobenzylphosphonate 20826-04-4, 5-Bromonicotinic acid 20980-22-7, 1-(2-Pyrimidyl)piperazine 23462-75-1, Tetrahydropyran-3-one 24252-37-7, Ethyl 1-methylpiperidine-4-carboxylate 25808-30-4 28611-39-4 29943-42-8, 4H-Tetrahydropyran-4-one 31252-42-3, 4-Benzylpiperidine 32231-06-4, 1-(3,4-Methylenedioxybenzyl)-piperazine 35386-24-4, 1-(2-Methoxyphenyl)piperazine 38212-30-5, 1-(4-Methoxyphenyl)piperazine 50541-93-0, 4-Amino-1-benzylpiperidine 50729-68-5 52146-35-7, 1-(3,4,5-Trimethoxybenzyl)piperazine 60548-09-6, 1-(2-Furoyl)piperazine hydrochloride 61081-32-1 73579-08-5, 1-Methyl-4-methylaminopiperidine 79099-07-3 80670-21-9 82261-42-5, 3-(4-Aminophenyl)pyridine 85199-06-0 87779-78-0 89878-14-8, Diethyl-(3-pyridyl)-borane 93777-26-5, 5-Bromo-2-fluorobenzaldehyde 96251-92-2 98546-51-1, 4-Methylthiophenylboronic acid 128796-39-4, 4-Trifluoromethylphenylboronic acid 162210-31-3 162271-10-5 175394-06-6 186498-02-2 229009-38-5 229009-39-6 229009-40-9 229009-41-0 229009-42-1 229009-43-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 623-04-1P, 4-Aminobenzyl alcohol 955-44-2P 2089-33-0P 2439-56-7P 4519-78-2P, Benzyldiethylphosphine oxide 5339-15-1P 6149-46-8P 6406-74-2P 6425-46-3P 6763-91-3P 6881-57-8P, Benzylphosphonic acid 14473-91-7P 15084-55-6P 15115-76-1P 15184-96-0P 16341-77-8P 17302-46-4P 18483-99-3P 18484-05-4P 20173-88-0P 20712-12-3P 22009-38-7P, 7-Hydroxy-1-tetralone 22237-13-4P, 4-Ethoxyphenylboronic acid 24100-18-3P 29124-57-0P 29608-05-7P 34035-05-7P 34160-40-2P 38035-10-8P 40594-34-1P 41526-73-2P, 7-Phenyl-1-tetralone

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79909-21-0P 83619-74-3P 91150-58-2P 91953-92-3P 92033-77-7P
93138-55-7P 94839-07-3P 95323-86-7P 98008-66-3P 123324-71-0P,
4-tert-Butylphenylboronic acid 131230-76-7P 133851-67-9P
135605-97-9P 138007-25-7P 139301-27-2P, 4-
Trifluoromethoxyphenylboronic acid 142335-64-6P 143632-57-9P
144464-65-3P 145654-38-2P 147539-41-1P 160127-63-9P 162607-15-0P
162607-20-7P 168897-21-0P 175393-25-6P 175394-17-9P 175840-02-5P
179055-22-2P 183608-47-1P 185111-27-7P 229006-54-6P 229006-55-7P
229006-56-8P 229006-57-9P 229006-58-0P 229006-59-1P 229006-60-4P
229006-61-5P 229006-62-6P 229006-63-7P 229006-64-8P 229006-65-9P
229006-66-0P 229006-67-1P 229006-68-2P 229006-69-3P 229006-70-6P
229006-71-7P 229006-72-8P 229006-73-9P 229006-74-0P 229006-75-1P
229006-76-2P 229006-77-3P 229006-78-4P 229006-79-5P 229006-80-8P
229006-81-9P 229006-82-0P 229006-83-1P 229006-84-2P 229006-85-3P
229006-86-4P 229006-87-5P 229006-88-6P 229006-89-7P 229006-90-0P
229006-91-1P 229006-92-2P 229006-93-3P 229006-94-4P 229006-95-5P
229006-96-6P 229006-97-7P 229006-98-8P 229006-99-9P 229007-00-5P
229007-01-6P 229007-02-7P 229007-03-8P 229007-04-9P 229007-05-0P
229007-06-1P 229007-07-2P 229007-08-3P 229007-09-4P 229007-10-7P
229007-11-8P 229007-12-9P 229007-13-0P 229007-14-1P 229007-15-2P
229007-16-3P 229007-17-4P 229007-18-5P 229007-19-6P 229007-20-9P
229007-21-0P 229007-22-1P 229007-23-2P 229007-24-3P 229007-25-4P
229007-26-5P 229007-27-6P 229007-28-7P 229007-29-8P 229007-30-1P
229007-31-2P 229007-32-3P 229007-33-4P 229007-34-5P 229007-35-6P
229007-36-7P 229007-37-8P 229007-38-9P 229007-39-0P 229007-40-3P
229007-41-4P 229007-42-5P 229007-43-6P 229007-44-7P 229007-45-8P
229007-46-9P 229007-47-0P 229007-48-1P 229007-49-2P 229007-50-5P
229007-51-6P 229007-52-7P 229007-53-8P 229007-54-9P 229007-55-0P
229007-56-1P 229007-57-2P 229007-58-3P 229007-59-4P 229007-60-7P
229007-61-8P 229007-62-9P 229007-63-0P 229007-64-1P 229007-65-2P
229007-66-3P 229007-67-4P 229007-68-5P 229007-69-6P 229007-70-9P
229007-71-0P 229007-72-1P 229007-73-2P 229007-74-3P 229007-75-4P
229007-76-5P 229007-77-6P 229007-78-7P 229007-79-8P 229007-80-1P
229007-81-2P 229007-82-3P 229007-83-4P 229007-84-5P 229007-85-6P
229007-86-7P 229007-87-8P 229007-88-9P 229007-89-0P 229007-90-3P
229007-91-4P 229007-92-5P 229007-93-6P 229007-94-7P 229007-95-8P
229007-96-9P 229007-97-0P 229007-98-1P 229007-99-2P 229008-00-8P
229008-01-9P 229008-02-0P 229008-03-1P 229008-04-2P 229008-05-3P
229008-06-4P 229008-07-5P 229008-09-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT 229008-11-1P 229008-14-4P 229008-16-6P 229008-18-8P 229008-20-2P
229008-22-4P 229008-24-6P 229008-26-8P 229008-27-9P 229008-28-0P
229008-29-1P 229008-30-4P 229008-31-5P 229008-32-6P 229008-33-7P
229008-34-8P 229008-35-9P 229008-36-0P 229008-37-1P 229008-38-2P
229008-39-3P 229008-40-6P 229008-41-7P 229008-42-8P 229008-43-9P
229008-44-0P 229008-45-1P 229008-46-2P 229008-47-3P 229008-48-4P
229008-49-5P 229008-50-8P 229008-51-9P 229008-52-0P 229008-53-1P
229008-54-2P 229008-55-3P **229008-56-4P**
229008-57-5P 229008-58-6P 229008-59-7P 229008-60-0P
229008-61-1P 229008-62-2P 229008-63-3P 229008-64-4P 229008-65-5P
229008-66-6P 229008-67-7P 229008-68-8P 229008-69-9P 229008-70-2P
229008-71-3P 229008-72-4P 229008-73-5P 229008-74-6P 229008-75-7P
229008-76-8P 229008-77-9P 229008-78-0P 229008-79-1P 229008-80-4P
229008-81-5P 229008-82-6P 229008-83-7P 229008-84-8P 229008-85-9P

229008-86-0P 229008-87-1P 229008-88-2P 229008-89-3P 229008-90-6P
229008-91-7P 229008-92-8P 229008-93-9P 229008-94-0P 229008-95-1P
229008-96-2P 229008-97-3P 229008-98-4P 229008-99-5P 229009-00-1P
229009-01-2P 229009-02-3P 229009-03-4P 229009-04-5P 229009-05-6P
229009-06-7P 229009-07-8P 229009-08-9P 229009-09-0P 229009-10-3P
229009-11-4P 229009-12-5P 229009-13-6P 229009-14-7P 229009-15-8P
229009-16-9P 229009-17-0P 229009-18-1P 229009-19-2P 229009-20-5P
229009-21-6P 229009-22-7P 229009-23-8P 229009-24-9P 229009-25-0P
229009-26-1P 229009-27-2P 229009-28-3P 229009-29-4P 229009-30-7P
229009-31-8P 229009-32-9P 229009-33-0P 229009-34-1P 229009-35-2P
229009-36-3P 229009-37-4P 229153-66-6P 229153-67-7P 229153-68-8P
229153-69-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

IT **229006-01-3P 229006-02-4P 229006-06-8P 229006-08-0P 229006-12-6P**

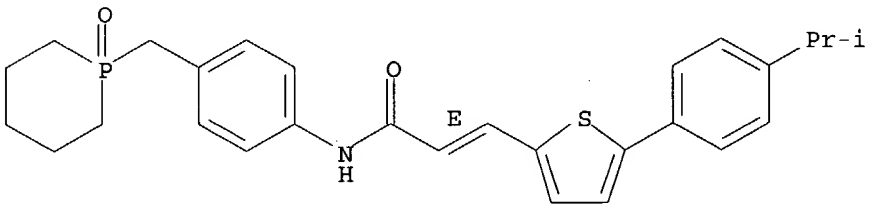
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides, naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

RN 229006-01-3 HCAPLUS

CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

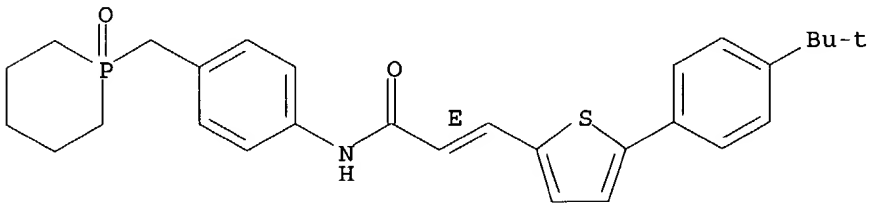
Double bond geometry as shown.



RN 229006-02-4 HCAPLUS

CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[(1-oxido-1-phosphorinanyl)methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

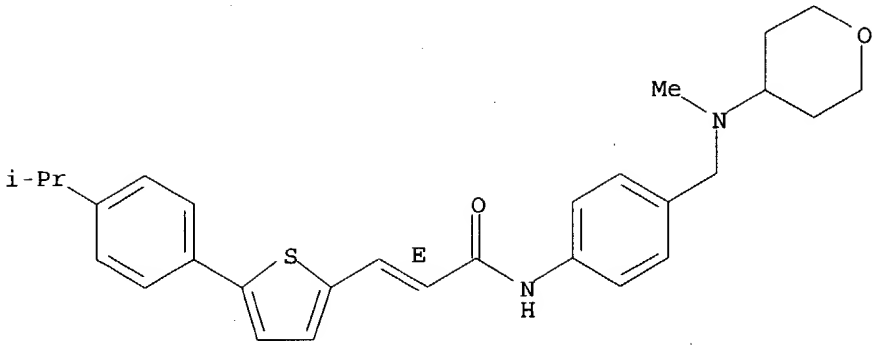
Double bond geometry as shown.



RN 229006-06-8 HCAPLUS

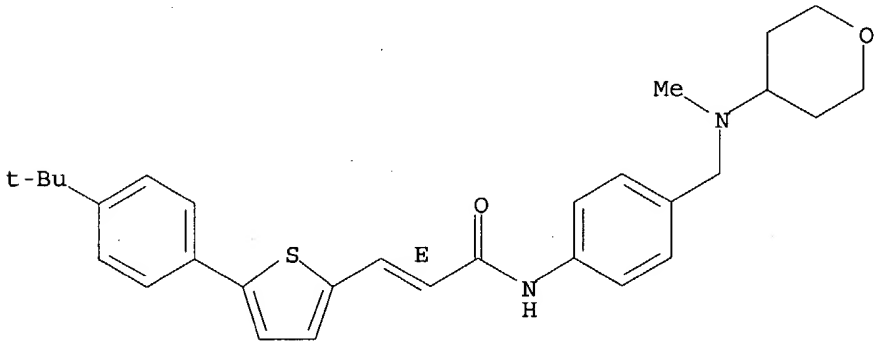
CN 2-Propenamide, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



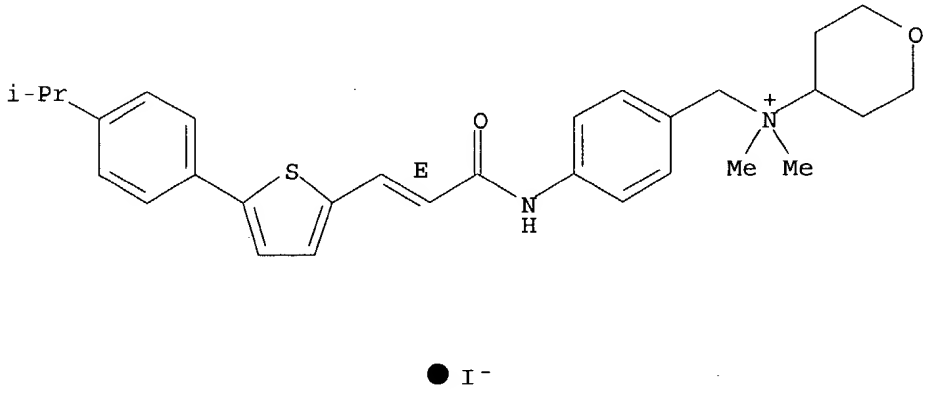
RN 229006-08-0 HCAPLUS
CN 2-Propenamide, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-N-[4-[[methyl(tetrahydro-2H-pyran-4-yl)amino]methyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 229006-12-6 HCAPLUS
CN 2H-Pyran-4-aminium, tetrahydro-N,N-dimethyl-N-[[4-[[(2E)-3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-1-oxo-2-propenyl]amino]phenyl]methyl]-, iodide (9CI) (CA INDEX NAME)

Double bond geometry as shown.



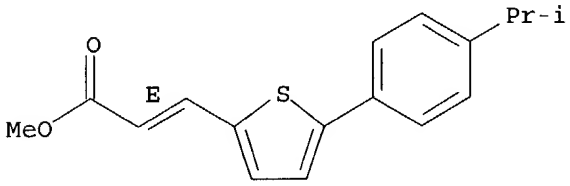
● I⁻

IT **229008-54-2P 229008-56-4P 229008-57-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzoxepinecarboxamides, benzocycloheptenecarboxamides,

naphthalenecarboxamides, and related compds. as MCP-1 receptor antagonists)

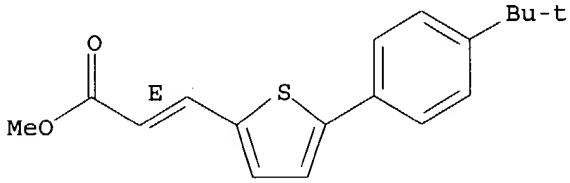
RN 229008-54-2 HCAPLUS
CN 2-Propenoic acid, 3-[5-[4-(1-methylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



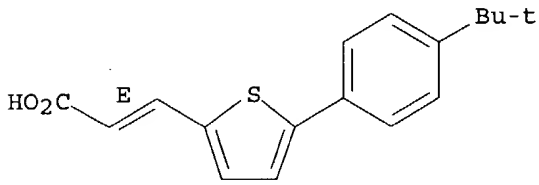
RN 229008-56-4 HCAPLUS
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

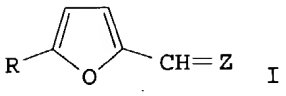


RN 229008-57-5 HCAPLUS
CN 2-Propenoic acid, 3-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L48 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:552173 HCAPLUS
DN 113:152173
ED Entered STN: 27 Oct 1990
TI Arylation of furanoid compounds with aryldiazonium salts
AU Obushak, N. D.; Ganushchak, N. I.; Lesyuk, A. I.; Dzikovskaya, L. M.; Kisilitsa, P. P.
CS L'vov. Gos. Univ., Lvov, USSR
SO Zhurnal Organicheskoi Khimii (1990), 26(4), 873-80
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
OS CASREACT 113:152173
GI



I

AB Condensation reaction of arylfurfurals I (R = Ph, 4-MeOC6H4, 4-ClC6H4, 4-O2NC6H4, 2- and 4-BrC6H4, 4-tolyl, 1-naphthyl; Z = O) with CH2(CO2H)2 in refluxing pyridine containing piperidine gave 58-92% furylacrylic acids I (Z = CHCO2H-E), which were arylated with R1N2+ Cl- (R1 = Ph, 4-ClC6H4, 2- and 4-BrC6H4, 4-O2NC6H4, 4-EtO2CC6H4) in aqueous Me2CO containing NaOAc and CuCl2 to 8 I (Z = CHR1-E) (II) in 27-54% yield. II were also prepared in 16-40% yield along with 17-32% I (Z = CHO-E) by arylating 3-(2-furyl)acrolein as above. I (R = Ph, 4-ClC6H4; Z = CHCHO-E) were also formed in 40-50% yield by treating I (Z = O) with MeCHO in H2O-CH2Cl2 containing NaOH and BuNEt3+ Cl-.

ST arylation furan deriv diazonium salt; styrylfuran furylacrolein prepn UV NMR; furylacrylic acid prepn arylation; acrylic acid furyl prepn arylation; acrolein furyl prepn UV NMR

IT Nuclear magnetic resonance
Ultraviolet and visible spectra
(of (arylfuryl)acroleins and arylstyrylfurans)

IT Arylation
(of furanoid compds. with aryldiazonium salts)

IT Diazonium compounds
RL: RCT (Reactant); RACT (Reactant or reagent)
(arene, salts, arylation by, of furanoid compds.)

IT 2028-79-7, 4-(Ethoxycarbonyl)phenyldiazonium chloride 2028-85-5, 4-Bromophenyldiazonium chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(arylation by, of (arylfuryl)acrylic acids)

IT 100-05-0 100-34-5 2028-74-2, 4-Chlorophenyldiazonium chloride 4346-59-2, 4-Methoxyphenyldiazonium chloride 34835-57-9, 2-Bromophenyldiazonium chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(arylation by, of furylacrolein and (arylfuryl)acrylic acids)

IT 623-30-3, 3-(2-Furyl)acrolein
RL: RCT (Reactant); RACT (Reactant or reagent)
(arylation of, with aryldiazonium chlorides)

IT 75-07-0, Acetaldehyde, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with arylfurfurals, (arylfuryl)acroleins by)

IT 141-82-2, Propanedioic acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with arylfurfurals, (arylfuryl)acrylic acids by)

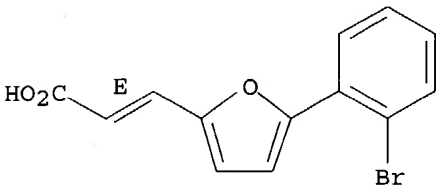
IT 7147-77-5, 5-(4-Nitrophenyl)furfural 13803-39-9, 5-Phenylfurfural 20005-42-9, 5-(4-Bromophenyl)furfural 34035-03-5, 5-(4-Chlorophenyl)furfural 34035-05-7, 5-(4-Tolyl)furfural 34070-33-2, 5-(4-Methoxyphenyl)furfural 51792-36-0 58110-57-9, 5-(2-Bromophenyl)furfural
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with malonic acid, (arylfuryl)acrylic acid by)

IT 62806-31-9P 62806-32-0P 62806-33-1P 62806-34-2P 62806-35-3P 62806-39-7P **129626-52-4P** 129626-62-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and arylation of, with aryldiazonium salts)

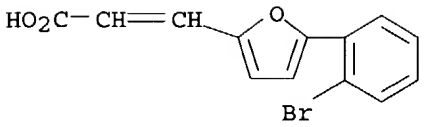
IT 40025-25-0P 104431-32-5P 108576-24-5P 129626-53-5P 129626-54-6P 129626-55-7P 129626-56-8P 129626-57-9P 129626-58-0P 129626-59-1P

129626-60-4P 129626-61-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **129626-52-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and arylation of, with aryldiazonium salts)
RN 129626-52-4 HCAPLUS
CN 2-Propenoic acid, 3-[5-(2-bromophenyl)-2-furanyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

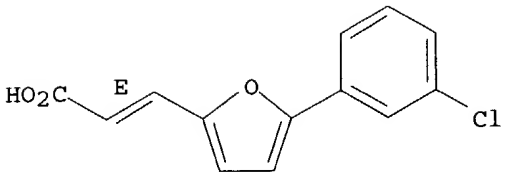


L48 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1988:510184 HCAPLUS
DN 109:110184
ED Entered STN: 01 Oct 1988
TI Synthesis of substituted furylacrylic acids and their chlorides
AU Lesyuk, A. I.; Dzikovskaya, L. M.; Obushak, N. D.; Ganushchak, N. I.
CS USSR
SO Vestn. L'vov. Un-ta. Ser. Khim. (1987), (28), 82-6
From: Ref. Zh., Khim. 1987, Abstr. No. 22Zh168
DT Journal
LA Russian
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
OS CASREACT 109:110184
AB Title only translated.
ST arylfurfuryl alc Knoevenagel condensation malonate; furylacrylic acid prepn chlorination; furylacryloyl chloride
IT Knoevenagel reaction
(of arylfurfuryl alcs. with malonic acid, furylacrylic acid by)
IT 141-82-2, Malonic acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(Knoevenagel reaction of, with arylfurfuryl alcs.)
IT 7147-77-5 13803-39-9 20005-42-9 34035-03-5 34035-05-7 34070-33-2 58110-57-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(Knoevenagel reaction of, with malonic acid)
IT 58110-37-5P 58110-42-2P 58110-43-3P 58110-44-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to acid chloride)
IT 58110-34-2P 58110-40-0P **58110-41-1P** 116218-06-5P 116218-07-6P 116218-08-7P 116218-09-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **58110-41-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 58110-41-1 HCAPLUS
CN 2-Propenoic acid, 3-[5-(2-bromophenyl)-2-furanyl]- (9CI) (CA INDEX NAME)

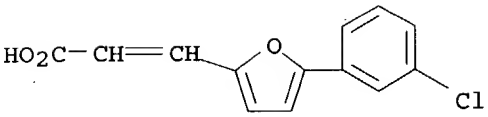


L48 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1977:188948 HCAPLUS
DN 86:188948
ED Entered STN: 12 May 1984
TI Transmission of substituent effects across the furan ring
AU Beno, A.; Krutosikova, A.
CS Dep. Anal. Chem., Comenius Univ., Bratislava, Czech.
SO Collection of Czechoslovak Chemical Communications (1977), 42(2), 508-11
CODEN: CCCCAK; ISSN: 0010-0765
DT Journal
LA English
CC 22-8 (Physical Organic Chemistry)
AB The half-wave potential values, apparent dissociation consts., and wavenos. of IR bands of 9 substituted 3-(5-phenyl-2-furyl)acrylic acids and 8 substituted cinnamic acids were correlated with σ substituent consts. The transmission coeffs. across the furan ring, π', were calculated from the obtained reaction consts. ρ and compared with the values of π' found for other systems. There was good agreement between the results obtained by different methods., and between the present and previous results (Beno, A., et al., 1973).
ST furanacrylic acid Hammett LFER; cinnamic acid Hammett LFER; acid cinnamic furanacrylic Hammett; substituent cinnamic furanacrylic acid; IR cinnamic furanacrylic acid; polarog cinnamic furanacrylic acid
IT Dissociation
Infrared spectra
Polarography
(of furyl- and phenylacrylic acids)
IT Substituent effect
(on properties of cinnamic and furanacrylic acids)
IT Linear free energy relationship
(Hammett, of furyl- and phenylacrylic acids)
IT 940-61-4 940-62-5 7312-27-8 14473-90-6 14737-89-4 17570-26-2
20595-30-6 62806-31-9 62806-32-0 62806-33-1 62806-34-2
62806-35-3 62806-37-5 62806-38-6
RL: PRP (Properties)
(dissociation, polarog., and IR of, Hammett relationship of)
IT 140-10-3, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(dissociation, polarog., and IR of, Hammett relationshp of)
IT **62806-36-4** 62806-39-7
RL: PRP (Properties)
(dissociation, polarog.,and IR of, Hammett relationship of)
IT **62806-36-4**
RL: PRP (Properties)
(dissociation, polarog.,and IR of, Hammett relationship of)
RN 62806-36-4 HCAPLUS
CN 2-Propenoic acid, 3-[5-(3-chlorophenyl)-2-furanyl]-, (E)- (9CI) (CA INDEX NAME)

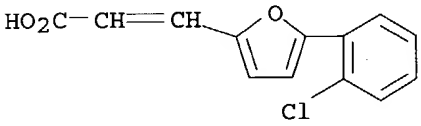
Double bond geometry as shown.



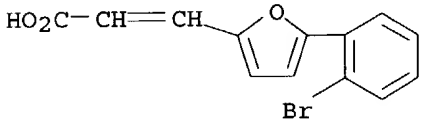
L48 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:58390 HCAPLUS
DN 84:58390
ED Entered STN: 12 May 1984
TI Furan derivatives. LXIII. Substituted 3-(5-phenyl-2-furyl)acrylic acids and their methyl esters. Transmission of polar effects across the furan-ethene system
AU Krutosikova, A.; Sura, J.; Kovac, J.; Juhas, S.
CS Dep. Org. Chem., Slovak Inst. Technol., Bratislava, Czech.
SO Collection of Czechoslovak Chemical Communications (1975), 40(11), 3362-9
CODEN: CCCCAK; ISSN: 0010-0765
DT Journal
LA English
CC 22-8 (Physical Organic Chemistry)
AB Thirteen 3-(5-phenyl-2-furyl)acrylic acids (unsubstituted or substituted by NO2, Cl, Br, Me, MeO, or CF3) were prepared by Perkin condensation of the corresponding furancarboxaldehydes. The apparent pKa values of the acids in 80% methyl cellosolve and the rate consts. kh of the alkaline hydrolysis of their Me esters in 60% aqueous Me2CO were determined potentiometrically. The obtained values are correlated with σ substituent consts. and the transmission of the polar effects of the substituents across the furan-ethene system is discussed.
ST phenylfuranacrylic acid dissocn const; hydrolysis const phenylfuranacrylate; polar effect phenylfuranacrylate; Hammet phenylfuranacrylate; furanacrylate phenyl polar effect; acrylate phenylfuryl polar effect
IT Dissociation
(consts., of phenylfuranacrylic acids)
IT Kinetics of hydrolysis
(of methyl phenylfuranacrylates)
IT Substituent effect
(on dissociation of phenylfuranacrylic acids or hydrolysis of their methyl esters)
IT 7147-77-5 13148-43-1 13803-39-9 20000-96-8 20005-42-9 22078-59-7
34035-03-5 34035-04-6 34035-05-7 34070-33-2 52130-30-0
58110-57-9 58110-58-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(Perkin reaction of)
IT 58110-34-2P 58110-35-3P 58110-36-4P 58110-37-5P **58110-38-6P**
58110-39-7P 58110-40-0P **58110-41-1P** 58110-42-2P
58110-43-3P 58110-44-4P 58110-45-5P 58110-46-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and dissociation constant of)
IT 58110-47-7P 58110-48-8P 58110-49-9P 58110-50-2P **58110-51-3P**
58110-52-4P 58110-53-5P 58110-54-6P 58110-55-7P 58110-56-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and hydrolysis constant of)
IT **58110-38-6P 58110-39-7P 58110-41-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and dissociation constant of)
RN 58110-38-6 HCAPLUS
CN 2-Propenoic acid, 3-[5-(3-chlorophenyl)-2-furanyl]- (9CI) (CA INDEX NAME)



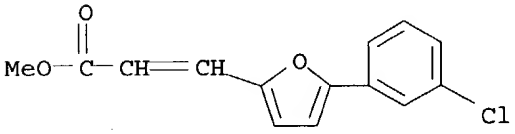
RN 58110-39-7 HCAPLUS
CN 2-Propenoic acid, 3-[5-(2-chlorophenyl)-2-furanyl]- (9CI) (CA INDEX NAME)



RN 58110-41-1 HCAPLUS
CN 2-Propenoic acid, 3-[5-(2-bromophenyl)-2-furanyl]- (9CI) (CA INDEX NAME)



IT **58110-51-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and hydrolysis constant of)
RN 58110-51-3 HCAPLUS
CN 2-Propenoic acid, 3-[5-(3-chlorophenyl)-2-furanyl]-, methyl ester (9CI)
(CA INDEX NAME)



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L47 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:455007 HCAPLUS
DN 131:194472
ED Entered STN: 26 Jul 1999
TI Quantitative structure-activity relationship studies of RAR α, β, γ retinoid agonists
AU Douguet, Dominique; Thoreau, Etienne; Grassy, Gerard
CS Centre International Recherches Dermatologie **GALDERMA**, Sophia Antipolis, F-06902, Fr.
SO Quantitative Structure-Activity Relationships (1999), 18(2), 107-123
CODEN: QSARDI; ISSN: 0931-8771
PB Wiley-VCH Verlag GmbH
DT Journal
LA English
CC 2-2 (Mammalian Hormones)

AB Structure-activity relationships were established for 140 synthetic retinoid agonists. Retinoids, natural and synthetic analogs of vitamin A, are activating ligands for retinoic acid receptors (RARα, β, and γ), members of the nuclear receptor superfamily. A QSAR study provides information on the type of intermol. and intramol. interactions the active mols. are exposed to during the course of their interaction with the receptor. Retinoid structures were modeled both by mol. and quantum mechanics and were submitted to a preliminary conformational anal. based on mol. dynamics. Linear and non-linear multivariate analyses were performed, revealing the principal electronic and structural characteristics leading to good affinity for each RAR subtype. Distinct structural features were found for each subtype: this is in agreement with the fact that the selectivity of the RAR subtypes results from the change of amino acids in the ligand cavity. Indeed, these amino-acids induce subtle changes in terms of steric properties and specific interactions, thus engendering specificity. The predictive ability of these relationships was validated using a large set of compds. which were not used to derive the model. The goal this of work was to detect relationships between structures and affinity for a broad range of retinoids in order that this model could be used in a more general manner, for example to impose constraints in database searching, or for use in automatic structure generation software.

ST retinoid structure activity relationship mol modeling; retinoic acid receptor QSAR

IT Drug design
Molecular modeling
QSAR (structure-activity relationship)
(QSAR studies of retinoic acid receptors α, β, γ retinoid agonists)

IT Retinoic acid receptors
Retinoids
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR studies of retinoic acid receptors α, β, γ retinoid agonists)

IT Retinoic acid receptors
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(RAR-α; QSAR studies of retinoic acid receptors α, β, γ retinoid agonists)

IT Retinoic acid receptors
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(RAR-β; QSAR studies of retinoic acid receptors α, β, γ retinoid agonists)

IT Retinoic acid receptors
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(RAR-γ; QSAR studies of retinoic acid receptors α, β, γ retinoid agonists)

IT 71441-28-6, Ttnpb 86471-16-1 94497-51-5, AM 80 99660-54-5
99660-64-7 102121-60-8, Am580 104224-10-4 104224-38-6 104224-43-3
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110952-22-2 110952-26-6 111008-33-4 116372-01-1 117168-45-3
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241140-34-1 241140-35-2 241140-36-3
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR studies of retinoic acid receptors α, β, γ retinoid agonists)

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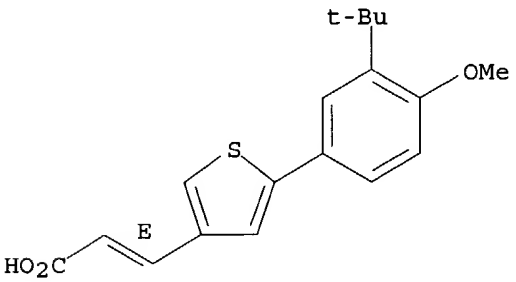
IT **241140-32-9 241140-33-0**
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR studies of retinoic acid receptors α, β, γ retinoid agonists)

RN 241140-32-9 HCAPLUS
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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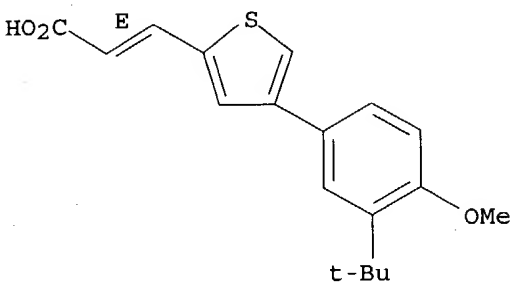
Double bond geometry as shown.



L47 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:623162 HCAPLUS
DN 127:293119
ED Entered STN: 29 Sep 1997
TI Preparation of bicyclic aromatic compounds
IN **Bernardon, Jean-Michel**
PA Centre International De Recherches Dermatologiques **Galderma**
(C.I.R.D. Galder, Fr.; Bernardon, Jean-Michel
SO PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DT Patent
LA French
IC ICM C07D333-24
ICS C07D333-16; C07D307-54; C07D207-32; C07D213-55; C07C069-618;
A61K031-38; A61K031-19
CC 27-1 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 25, 62, 63
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9733881	A1	19970918	WO 1997-FR391	19970305 <--
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, GH, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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AU 704753	B2	19990506		
EP 832081	A1	19980401	EP 1997-908308	19970305 <--
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	US 1998-952804	A1	19980126			
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	US 2000-619582	A3	20000912			

OS MARPAT 127:293119

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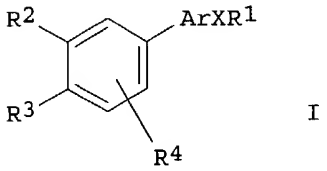


I

AB Novel bicyclic aromatic compds. I [R1 = Me, CH2OR5, COR6; Ar = = (un)substituted Ph, pyridyl, furyl, thienyl, pyrrolyl; X = CR8:CR9, C.tplbond.C; R2, R3 = H, alkyl, OR5, SR5; R2R3 = aromatic ring; R5 = H, alkyl, acyl; R6 = H, alkyl, NR'R''; R8, R9 = H, alkyl] and their use in pharmaceutical compns. useful in treatment of dermatol. conditions (no data) or their use in cosmetic compns. (no data) are disclosed. E.g., reaction of 3-tert-butyl-4-methoxyphenylboronic acid and 4-bromo-2-thiophenecarboxaldehyde gave 4-(3-tert-butyl-4-methoxyphenyl)-2-thiophenecarboxaldehyde. The last was treated with tri-Et phosphonoacetate to give Et 4-(3-tert-butyl-4-methoxyphenyl)-2-thiopheneacrylate. The ester was converted to the corresponding acid.

ST bicyclic arom compd prepn; naphthylthiopheneacrylic acid prepn; thiopheneacrylic acid naphthyl prepn; naphthylphenylpropiolic acid prepn; propiolic acid naphthylphenyl prepn; pyrrolylacrylic acid naphthyl prepn; dermatol agent bicyclic arom compd; cosmetic agent bicyclic arom compd

IT Aromatic compounds
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of bicyclic aromatic compds.)

IT Cosmetics
(preparation of bicyclic aromatic compds. as cosmetic agents)

IT Skin preparations (pharmaceutical)
(preparation of bicyclic aromatic compds. as dermatol. agents)

IT **196960-59-5P** 196960-60-8P **196960-61-9P**
196960-62-0P **196960-63-1P** **196960-64-2P**
196960-65-3P 196960-66-4P 196960-67-5P 196960-68-6P
196960-69-7P 196960-70-0P 196960-71-1P 196960-72-2P 196960-73-3P
196960-74-4P 196960-75-5P 196960-76-6P 196960-77-7P 196960-78-8P
196960-79-9P 196960-80-2P 196960-81-3P 196960-82-4P 196960-83-5P
196960-84-6P 196960-85-7P 196960-86-8P 196960-87-9P 196960-88-0P
196960-89-1P 196961-42-9P 196961-43-0P 196961-44-1P 196961-45-2P
196961-47-4P 196961-49-6P 196961-50-9P 196961-51-0P 196961-52-1P
196961-53-2P 196961-54-3P 196961-55-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of bicyclic aromatic compds.)

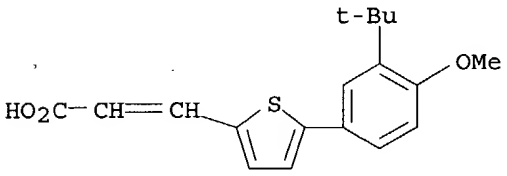
IT 99-90-1 108-40-7, 3-Methylthiophenol 110-91-8, Morpholine, reactions

123-30-8, 4-Hydroxyaniline 629-04-9, 1-Bromoheptane 870-63-3
931-33-9 1122-91-4, 4-Bromobenzaldehyde 1200-07-3 1761-61-1,
5-Bromo-2-hydroxybenzaldehyde 4701-17-1 14804-34-3 18791-75-8
27452-17-1 62224-19-5 119999-22-3 168082-64-2 170355-38-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bicyclic aromatic compds.)

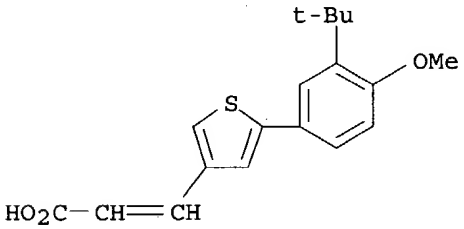
IT 33694-79-0P 135631-86-6P 158115-92-5P 168082-41-5P 169126-63-0P
169126-64-1P 170100-73-9P 189698-90-6P 189698-91-7P 189699-37-4P
191469-48-4P 196960-90-4P 196960-91-5P 196960-92-6P 196960-93-7P
196960-94-8P 196960-95-9P 196960-96-0P 196960-97-1P 196960-98-2P
196960-99-3P **196961-00-9P** 196961-01-0P **196961-02-1P**
196961-03-2P **196961-04-3P** 196961-05-4P **196961-06-5P**
196961-07-6P **196961-08-7P** 196961-09-8P 196961-10-1P
196961-11-2P 196961-12-3P 196961-13-4P 196961-14-5P 196961-15-6P
196961-16-7P 196961-17-8P 196961-18-9P 196961-19-0P 196961-20-3P
196961-21-4P 196961-22-5P 196961-23-6P 196961-24-7P 196961-25-8P
196961-26-9P 196961-27-0P 196961-28-1P 196961-29-2P 196961-30-5P
196961-31-6P 196961-32-7P 196961-33-8P 196961-34-9P 196961-35-0P
196961-36-1P 196961-37-2P 196961-38-3P 196961-39-4P 196961-40-7P
196961-41-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bicyclic aromatic compds.)

IT **196960-59-5P 196960-61-9P 196960-62-0P**
196960-63-1P 196960-64-2P 196960-65-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of bicyclic aromatic compds.)

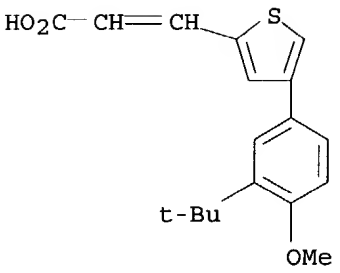
RN 196960-59-5 HCAPLUS
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]-(9CI) (CA INDEX NAME)



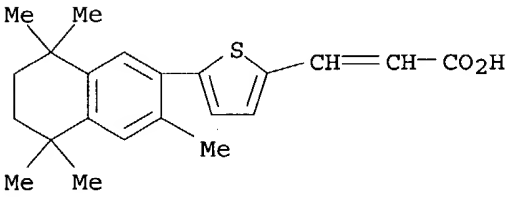
RN 196960-61-9 HCAPLUS
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]-(9CI) (CA INDEX NAME)



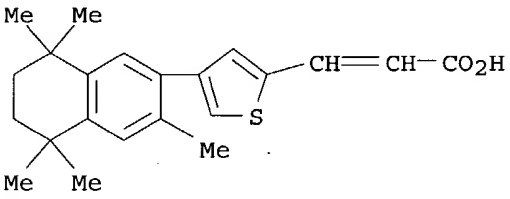
RN 196960-62-0 HCAPLUS
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]-(9CI) (CA INDEX NAME)



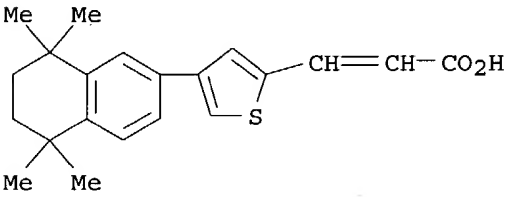
RN 196960-63-1 HCAPLUS
CN 2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)



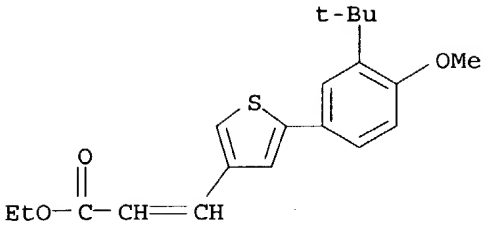
RN 196960-64-2 HCAPLUS
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)



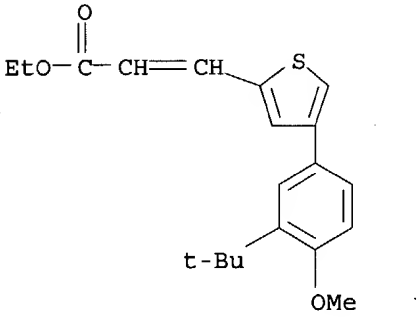
RN 196960-65-3 HCAPLUS
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-thienyl]- (9CI) (CA INDEX NAME)



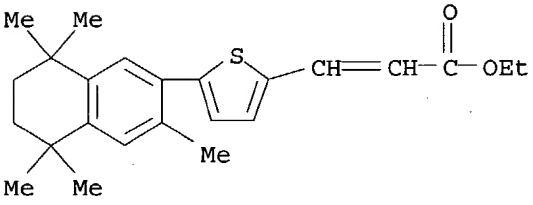
IT **196961-00-9P 196961-02-1P 196961-04-3P**
196961-06-5P 196961-08-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bicyclic aromatic compds.)
RN 196961-00-9 HCAPLUS
CN 2-Propenoic acid, 3-[5-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-3-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



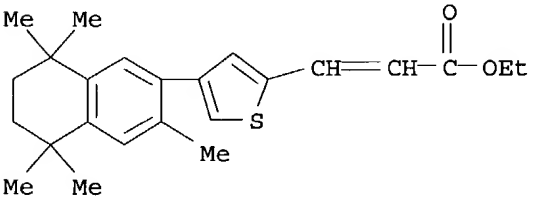
RN 196961-02-1 HCAPLUS
CN 2-Propenoic acid, 3-[4-[3-(1,1-dimethylethyl)-4-methoxyphenyl]-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



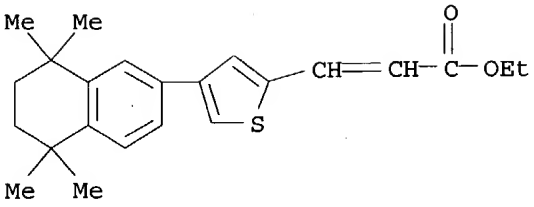
RN 196961-04-3 HCAPLUS
CN 2-Propenoic acid, 3-[5-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 196961-06-5 HCAPLUS
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 196961-08-7 HCAPLUS
CN 2-Propenoic acid, 3-[4-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-thienyl]-, ethyl ester (9CI) (CA INDEX NAME)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